US ERA ARCHIVE DOCUMENT

TABLE A-3-1
CHEMICAL-SPECIFIC INPUTS FOR ACENAPHTHENE (83-32-9)

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		154.21		
$T_m(K)$	Budavari, O'Neil, Smith, and Heckelman (1989)		368.1		
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).		4.93E-06 at 25°C (solid)		
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).		3.80E+00		
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.00E-04		
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.21E-02		
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.19E-06		
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).		9.22E+03		
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).		4.90E+03		
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.90E+01		
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.67E+02		

## TABLE A-3-1 CHEMICAL-SPECIFIC INPUTS FOR ACENAPHTHENE (83-32-9)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.96E+02
ksg (year) <sup>-1</sup>	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.48E+00
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $T_m$ and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
	<b>Biotransfer Factors for Plants</b>		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.69E+02
$Br_{root veg} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	5.48E+00
$Br_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.98E-01
$Br_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.98E-01
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for leafyaboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.66E+00

CHEMICAL-SPECIFIC INPUTS FOR ACENAPHTHENE (83-32-9)

Parameter	Reference and Explanation	Equations	Value
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.66E+00
	<b>Biotransfer Factors for Animals</b>		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	7.32E-05
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.31E-04
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.80E-04
Ba <sub>egg</sub> (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	7.32E-02
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.83E-04
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	6.07E+02
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	6.00E-02
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m³)	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	2.10E-01
Inhalation URF (μg/m³) <sup>-1</sup>		C-2-1	ND

#### CHEMICAL-SPECIFIC INPUTS FOR ACENAPHTHENE (83-32-9)

Parameter	Reference and Explanation	Equations	Value
Health Benchmarks (continued)			
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA = Not applicable ND = No data available

TABLE A-3-2
CHEMICAL-SPECIFIC INPUTS FOR ACETALDEHYDE (75-07-0)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)		44.05
$T_m(\mathbf{K})$	Montgomery and Welkom (1991)		149.6
Vp (atm)			ND
S (mg/L)			ND
H (atm·m³/mol)		B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.72E-01
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.33E-05
$K_{ow}$ (unitless)	Recommended $K_{ow}$ value cited in Karickhoff and Long (1995).		6.02E-01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	-	9.53E-01
K $d_s$ (cm³/g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.53E-03
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.15E-02
Kd <sub>bs</sub> (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.81E-02

## TABLE A-3-2 CHEMICAL-SPECIFIC INPUTS FOR ACETALDEHYDE (75-07-0)

Parameter	Reference and Explanation	Equations	Value	
Chemical/Physical Properties (Continued)				
ksg (year)-1	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0	
Fv (unitless)	Fv value was assumed to be 1.0 due to a lack of data.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0	
	<b>Biotransfer Factors for Plants</b>			
RCF $ (\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}) $	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.46E+00	
$Br_{root veg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	6.78E+02	
$Br_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	5.19E+01	
$Br_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	5.19E+01	
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$		B-2-8	ND	
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$		B-3-8	ND	

### CHEMICAL-SPECIFIC INPUTS FOR ACETALDEHYDE (75-07-0)

**TABLE A-3-2** 

Parameter	Reference and Explanation	Equations	Value	
	Biotransfer Factors for Animals			
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	4.78E-09	
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.51E-08	
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.83E-08	
Ba <sub>egg</sub> (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	4.78E-06	
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.19E-08	
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.00E-01	
BAF <sub>fish</sub> (L/kg FW)	-	B-4-27	NA	
$BSAF_{fish}$ (unitless)	-	B-4-28	NA	
	Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1996d)	C-1-8	2.6E-03	
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1996d)	C-1-7	7.7E-03	
RfC (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	9.00E-03	
Inhalation URF (μg/m³) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	2.20E-06	
Inhalation CSF (mg/kg/day) <sup>-1</sup>	Value based on <i>Oral CSF</i> assuming route-to-route extrapolation.	C-2-2	7.70E-03	

Note:

NA = Not applicable ND = No data available

# TABLE A-3-3 CHEMICAL-SPECIFIC INPUTS FOR ACETONE (67-64-1)

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		58.08		
$T_m(K)$	Budavari, O'Neil, Smith, and Heckelman (1989)		179.1		
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).		2.99E-01 at 25°C (liquid)		
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).		6.04E+05		
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.88E-05		
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.87E-01		
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.15E-05		
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994g).		6.00E-01		
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		9.51E-01		
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.51E-03		
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.13E-02		
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.80E-02		

# TABLE A-3-3 CHEMICAL-SPECIFIC INPUTS FOR ACETONE (67-64-1)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
ksg (year) <sup>-1</sup>	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
	Biotransfer Factors for Plants		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.46E+00
$Br_{root  veg} = \frac{(\mu g/g  DW  plant)}{\mu g/g  soil}$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	6.80E+02
$Br_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produceand forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	5.20E+01
$Br_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegorund and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	5.20E+01
$Bv_{ag} = \frac{(\mu g/g \ DW \ plant)}{\mu g/g \ air}$	$Bv_{leafy\ veg}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for abovegorund produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.13E-03
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.13E-03

## TABLE A-3-3 CHEMICAL-SPECIFIC INPUTS FOR ACETONE (67-64-1)

Parameter	Reference and Explanation	Equations	Value		
	Biotransfer Factors for Animals				
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	4.77E-09		
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.51E-08		
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.82E-08		
Ba <sub>egg</sub> (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	4.77E-06		
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.19E-08		
BCF <sub>fish</sub> (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF$ values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	4.00E-01		
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA		
$BSAF_{fish}$ (unitless)		B-4-28	NA		
	Health Benchmarks				
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	1.00E-01		
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND		
RfC (mg/m³)	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.50E-01		
Inhalation URF (µg/m³) <sup>-1</sup>		C-2-1	ND		
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND		

Note:

NA = Not applicable

ND = No data available

CHEMICAL-SPECIFIC INPUTS FOR ACETONITRILE (75-05-8)

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		41.05		
$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)		318.1		
Vp (atm)	Howard (1989-1993)		1.20E-01 at 25°C (solid)		
S (mg/L)	Howard (1989-1993)		1.30E-01		
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.79E+01		
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.14E-01		
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.40E-05		
$K_{ow}$ (unitless)	$\log K_{ow}$ value cited in Karickhoff and Long (1995).		4.57E-01		
K <sub>oc</sub> (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		7.69E-01		
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.69E-03		
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.76E-02		
Kd <sub>bs</sub> (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.07E-02		

## TABLE A-3-4 CHEMICAL-SPECIFIC INPUTS FOR ACETONITRILE (75-05-8)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
ksg (year) <sup>-1</sup>	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $T_m$ and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
	Biotransfer Factors for Plants		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The valus was then converted to a dry wight basis by using a moisture content of 87 percent.	B-2-10	6.43E+00
$Br_{root  veg} = \frac{(\mu g/g  DW  plant)}{\mu g/g  soil}$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	8.37E+02
$Br_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegrouns produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	6.09E+01
$Br_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegorund produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	6.09E+01
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	6.41E-10
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	6.41E-10

TABLE A-3-4

CHEMICAL-SPECIFIC INPUTS FOR ACETONITRILE (75-05-8)

Parameter	Reference and Explanation	Equations	Value		
	Biotransfer Factors for Animals				
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.63E-09		
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.15E-08		
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.39E-08		
Ba <sub>egg</sub> (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.63E-06		
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	9.06E-09		
BCF <sub>fish</sub> (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.25E-01		
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA		
$BSAF_{fish}$ (unitless)		B-4-28	NA		
	Health Benchmarks				
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	6.00E-03		
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND		
RfC (mg/m³)	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	2.10E-02		
Inhalation URF (μg/m³)-1		C-2-1	ND		
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND		

Note:

NA = Not applicable

ND = No data available

CHEMICAL-SPECIFIC INPUTS FOR ACETOPHENONE (98-86-2)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)		120.50
$T_m(K)$	Budavari, O'Neill, Smith, and Heckelman (1989)		293.6
Vp (atm)	Vp value cited in U.S. EPA (1995b).		5.20E-04 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1995b).		6.10E+03
<i>H</i> (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the <i>MW</i> , <i>S</i> , and <i>Vp</i> values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.03E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.00E-02
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.73E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).		4.37E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		2.69E+01
<i>Kd<sub>s</sub></i> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.69E-01
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.02E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.08E+00

CHEMICAL-SPECIFIC INPUTS FOR ACETOPHENONE (98-86-2)

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties (Continued)				
ksg (year) <sup>-1</sup>	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0		
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $T_m$ and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0		
	Biotransfer Factors for Plants				
RCF $ (\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}) $	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.06E+01		
$Br_{root veg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	3.92E+01		
$Br_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.37E+00		
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.37E+00		
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.04E-01		
$Bv_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.04E-01		

CHEMICAL-SPECIFIC INPUTS FOR ACETOPHENONE (98-86-2)

Parameter	Reference and Explanation	Equations	Value
	<b>Biotransfer Factors for Animals</b>		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.47E-07
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.10E-06
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.33E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.47E-04
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	8.66E-07
BCF <sub>fish</sub> (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.04E+01
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-01
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m³)	Calculated from <i>Oral RfD</i> using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	3.50E-01
<i>Inhalation URF</i> (μg/m³)-1		C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA= Not applicable ND= No data available

## TABLE A-3-6 CHEMICAL-SPECIFIC INPUTS FOR ACROLEIN (107-02-8)

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		56.06		
$T_m(K)$	Budavari, O'Neil, Smith, and Heckelman (1989)		185.1		
Vp (atm)	Vp value cited in U.S. EPA (1995b).		3.50E-01 at 25°C (liquid)		
S (mg/L)	S value cited in U.S. EPA (1995b).		2.10E+05		
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.34E-05		
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.92E-01		
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.22E-05		
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).		9.80E-01		
K <sub>oc</sub> (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		1.39E+00		
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.39E-02		
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.05E-01		
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	5.57E-02		

## TABLE A-3-6 CHEMICAL-SPECIFIC INPUTS FOR ACROLEIN (107-02-8)

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties (Continued)				
ksg (year)-1	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00		
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0		
	<b>Biotransfer Factors for Plants</b>				
RCF $ (\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}) $	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.54E+00		
$Br_{root veg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	4.69E+02		
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.92E+01		
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.92E+01		
$Bv_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	5.86E-04		
$Bv_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	5.86E-04		

### TABLE A-3-6 CHEMICAL-SPECIFIC INPUTS FOR ACROLEIN (107-02-8)

Parameter	Reference and Explanation	Equations	Value	
	Biotransfer Factors for Animals			
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	7.78E-09	
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.46E-08	
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.98E-08	
Ba <sub>egg</sub> (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	7.78E-06	
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.94E-08	
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	5.80E-01	
BAF <sub>fish</sub> (L/kg FW)	-	B-4-27	NA	
$BSAF_{fish}$ (unitless)		B-4-28	NA	
	Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	2.0E-02	
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND	
RfC (mg/m <sup>3</sup> )	U.S. EPA (1997)	C-2-3	2.0E-05	
Inhalation URF (μg/m³) <sup>-1</sup>		C-2-1	ND	
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND	

Note:

NA= Not applicable ND= No data available

TABLE A-3-7
CHEMICAL-SPECIFIC INPUTS FOR ACRYLONITRILE (107-13-1)

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		53.06		
$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)		189.6		
Vp (atm)	Vp value cited in U.S. EPA (1995b).		1.40E-01 at 25°C (liquid)		
S (mg/L)	S value cited in U.S. EPA (1995b).		7.50E+04		
<i>H</i> (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.90E-05		
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.11E-01		
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.23E-05		
K <sub>ow</sub> (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).		1.78E+00		
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		2.22E+00		
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.22E-02		
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.66E-01		
Kd <sub>bs</sub> (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	8.88E-02		

## TABLE A-3-7 CHEMICAL-SPECIFIC INPUTS FOR ACRYLONITRILE (107-13-1)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
ksg (year) <sup>-1</sup>	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.10E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
	<b>Biotransfer Factors for Plants</b>		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.67E+00
$Br_{root  veg} = \frac{(\mu g/g  DW  plant)}{\mu g/g  soil}$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	3.00E+02
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.77E+01
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.77E+01
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.04E-03
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.04E-03

### CHEMICAL-SPECIFIC INPUTS FOR ACRYLONITRILE (107-13-1)

**TABLE A-3-7** 

Parameter	Reference and Explanation	Equations	Value	
	Biotransfer Factors for Animals			
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.41E-08	
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	4.47E-08	
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	5.41E-08	
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.41E-05	
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	3.53E-08	
BCF <sub>fish</sub> (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF$ values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	4.80E+01	
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA	
$BSAF_{fish}$ (unitless)		B-4-28	NA	
	Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	1.0E-03	
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	5.4E-01	
RfC (mg/m³)	U.S. EPA (1997b)	C-2-3	2.0E-03	
Inhalation URF (μg/m³)-1	U.S. EPA (1997b)	C-2-1	6.8E-05	
Inhalation CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	2.4E-01	

Note:

NA= Not applicable ND= No data available

CHEMICAL-SPECIFIC INPUTS FOR ALDRIN (309-00-2)

Parameter	Reference and Explanation	Equations	Value	
Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		364.93	
$T_m(K)$	Budavari, O'Neil, Smith, and Heckelman (1989)		377.1	
Vp (atm)	Vp value cited in U.S. EPA (1992).		2.90E-11 at 25°C (solid)	
S (mg/L)	S value cited in U.S. EPA (1992).		7.84E-02	
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.35E-07	
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.43E-02	
$D_w$ (cm <sup>2</sup> /s)	$D_{w}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	4.40E-06	
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994f).		1.51E+06	
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).		4.87E+04	
<i>Kd</i> <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.87E+02	
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction oF 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.65E+03	
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.95E+03	

## TABLE A-3-8 CHEMICAL-SPECIFIC INPUTS FOR ALDRIN (309-00-2)

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties (Continued)				
ksg (year) <sup>-1</sup>	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	4.28E-01		
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $T_m$ and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.227		
	Biotransfer Factors for Plants				
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.33E+04		
$Br_{rootveg} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	2.73E+01		
$Br_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.04E-02		
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.04E-02		
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.58E+06		
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.58E+06		

#### CHEMICAL-SPECIFIC INPUTS FOR ALDRIN (309-00-2)

**TABLE A-3-8** 

Parameter	Reference and Explanation	Equations	Value
	<b>Biotransfer Factors for Animals</b>		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.20E-02
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.79E-02
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	4.59E-02
Ba <sub>egg</sub> (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.20E+01
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.99E-02
BCF <sub>fish</sub> (L/kg FW tissue)		B-4-26	NA
BAF <sub>fish</sub> (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.82E+05
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	3.00E-05
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997b)	C-1-7	1.70E+01
RfC (mg/m <sup>3</sup> )	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.10E-04
<i>Inhalation URF</i> (μg/m³) <sup>-1</sup>	U.S.EPA (1997b)	C-2-1	4.90E-03
Inhalation CSF (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997c)	C-2-2	1.70E+01

Note:

NA = Not applicable

ND = No data available

# TABLE A-3-9 CHEMICAL-SPECIFIC INPUTS FOR ANILINE (62-53-3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		93.12
$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)		266.8
Vp (atm)	Vp value cited in U.S. EPA (1995b).		8.80E-04 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).		3.60E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.28E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.56E-01
$D_w$ (cm <sup>2</sup> /s)	$D_{\rm w}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.01E-05
K <sub>ow</sub> (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).		9.55E+00
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		8.23E+00
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.23E-02
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.17E-01

### CHEMICAL-SPECIFIC INPUTS FOR ANILINE (62-53-3)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.29E-01
	Chemical/Physical Properties (Continued)		
ksg (year)-1	NC DEHNR (1996)	B-1-2; B-2-2; B-3-2; B-4-2	3.20E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
	Biotransfer Factors for Plants		
RCF $ (\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}) $	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	7.63E+00
$Br_{root veg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root  veg}$ value was calculated by dividing the <i>RCF</i> value with the $Kd_s$ value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	9.27E+01
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with i that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.05E+01
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.05E+01
$Bv_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of $25^{\circ}$ C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-9	2.72E-01

#### **CHEMICAL-SPECIFIC INPUTS FOR ANILINE (62-53-3)**

**TABLE A-3-9** 

Parameter	Reference and Explanation	Equations	Value
$Bv_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-9	2.72E-01
	<b>Biotransfer Factors for Animals</b>		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	7.59E-08
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.40E-07
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-12	2.90E-07
Ba <sub>eggs</sub> (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	7.59E-05
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.3 of Appendix A-3).	B-3-14	1.89E-07
BCF <sub>fish</sub> (L/kg, FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.27E+00
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1996d)	C-1-8	2.9E-04
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	5.7E-03
RfC (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	1.0E-03
<i>Inhalation URF</i> (μg/m³)-1	Calculated from <i>Oral CSF</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	1.6E-03
Inhalation CSF (mg/kg/day) <sup>-1</sup>	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	5.7E-03

Note:

$$\begin{split} NA &= Not \ applicable \\ ND &= No \ data \ available \\ All \ parameters \ are \ defined \ in \ list \ of \ FATE \ AND \ TRANSPORT \ PARAMETERS \ on \ page \ A-3-iii. \end{split}$$

## TABLE A-3-9 CHEMICAL-SPECIFIC INPUTS FOR ANILINE (62-53-3)

### CHEMICAL-SPECIFIC INPUTS FOR ANTHRACENE (120-12-7)

Parameter	Reference and Explanation	Equations	Value	
Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		178.22	
$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)		491.1	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)		3.35E-08 at 25°C (solid)	
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)		5.37E-02	
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.11E-04	
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.24E-02	
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.74E-06	
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c)		2.95E+04	
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).		2.35E+04	
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.35E+02	
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.76E+03	
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	9.40E+02	
	Chemical/Physical Properties (Continued)			
ksg (year) <sup>-1</sup>	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	5.50E-01	
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $T_m$ and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1;	1.0	

### CHEMICAL-SPECIFIC INPUTS FOR ANTHRACENE (120-12-7)

Parameter	Reference and Explanation	Equations	Value	
Biotransfer Factors for Plants				
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.49E+02	
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	2.76E+00	
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.01E-01	
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.01E-01	
$Bv_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.90E+01	
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.90E+01	
	<b>Biotransfer Factors for Animals</b>			
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.34E-04	
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	7.41E-04	
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	8.98E-04	
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.34E-01	
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	5.85E-04	

#### CHEMICAL-SPECIFIC INPUTS FOR ANTHRACENE (120-12-7)

Parameter	Reference and Explanation	Equations	Value
BCF <sub>fish</sub> (L/kg FW tissue)	_	B-4-26	NA
BAF <sub>fish</sub> (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCF$ s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCM$ s were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	2.60E+03
$BSAF_{fish}$ (unitless)	-	B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-01
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m³)	Calculated from $\it{RfD}$ using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.1E+00
Inhalation URF (μg/m³) <sup>-1</sup>		C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA= Not applicable; ND= No data available

## TABLE A-3-11 CHEMICAL-SPECIFIC INPUTS FOR ANTIMONY (7440-36-0)

Parameter	Reference and Explanation	Equations	Value	
Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		121.75	
$T_m$ (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)		903.1	
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.		0.0	
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.		NA	
H (atm·m³/mol)	${\cal H}$ value is assumed to be zero, because the ${\cal V}p$ and ${\cal S}$ values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0	
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.73E-02	
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	8.96E-06	
$K_{ow}$ (unitless)			NA	
$K_{oc}$ (mL/g)			NA	
Kd <sub>s</sub> (mL/g)	<i>Kd</i> <sub>s</sub> value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	45 at pH=6.8	
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	45 at pH=6.8	
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value is assumed to be same as the $Kd_{s}$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	45 at pH=6.8	
ksg (year) <sup>-1</sup>		B-1-2; B-2-2; B-3-2; B-4-2	ND	
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0	

Bapork (day/kg FW)

**TABLE A-3-11** 

CHEMICAL-SPECIFIC INPUTS FOR ANTIMONY (7440-36-0)

#### **Parameter** Reference and Explanation **Equations** Value **Biotransfer Factors for Plants** RCFB-2-10 ND $(\mu g/g \ DW \ plant)$ μg/mL soil water $Br_{rootveg}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjoreen, and $Br_{rootveg}$ B-2-10 3.00E-02 $(\mu g/g \ DW \ plant)$ Shor (1984) were used for $Br_{rootveg}$ . $\mu g/g$ soil $Br_{ag}$ value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). B-2-9 3.19E-02 $Br_{ag}$ Br values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and $(\frac{\mu g/g \ DW \ plant}{})$ Shor (1984) were used for Br<sub>ag</sub> (fruits). Br<sub>ag</sub> value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative (reproductive) growth and Bv values for vegetative $\mu g/g$ soil growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for $Br_{ag}$ (vegetables). The weighted average $Br_{ag}$ value for aboveground produce was obtained as follows: (1) $Br_{ag}$ values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) $Br_{ag}$ values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day. $Br_{forage}$ $Br_{forage}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Bv values for vegetative growth (such as leaves and stems) in Baes, Sharp, B-3-8 2.00E-01 $(\frac{\mu g/g \ DW \ plant}{})$ Sjoreen, and Shor (1984) were used for $Br_{forage}$ . $\mu g/g$ soil $Br_{grain}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth as recommended by Baes, Sharp, Sjoreen, and $Br_{grain}$ B-3-8 2.00E-01 $(\frac{\mu g/g \ DW \ plant}{})$ Shor (1984) were used for $Br_{erain}$ . $\mu g/g$ soil Metals are assumed to not experience air-to-leaf transfer, as cited in B-2-8 NA $Bv_{ag}$ U.S. EPA (1995b). $(\mu g/g \ DW \ plant)$ $\mu g/g$ air $Bv_{forage}$ B-3-8 NA Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b). $(\frac{\mu g/g \ DW \ plant}{})$ $\mu g/g$ air **Biotransfer Factors for Animals** Ba<sub>milk</sub> values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all 1.0E-04 Ba<sub>milk</sub> (day/kg FW) B-3-11 metals, except cadmium, mercury, selenium, and zinc. Babeef (day/kg FW) B-3-10 1.0E-03 Babeef values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc. **Biotransfer Factors for Animals (Continued)**

ND

B-3-12

### TABLE A-3-11 CHEMICAL-SPECIFIC INPUTS FOR ANTIMONY (7440-36-0)

Parameter	Reference and Explanation	Equations	Value
Ba <sub>egg</sub> (day/kg FW)		B-3-13	ND
Ba <sub>chicken</sub> (day/kg FW)		B-3-14	ND
BCF <sub>fish</sub> (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-4-26	4.00E+01
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1995d)	C-1-8	4.0E-04
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m³)	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.43E-03
Inhalation URF (μg/m³) <sup>-1</sup>		C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

### CHEMICAL-SPECIFIC INPUTS FOR AROCLOR 1016 (12674-11-2)

**TABLE A-3-12** 

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)		257.9
$T_m(\mathbf{K})$			ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).		9.37E-07 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).		5.71E-01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.23E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.69E-02
$D_w$ (cm <sup>2</sup> /s)	$D_{\rm w}$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	5.43E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).		2.53E+05
K <sub>oc</sub> (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		2.32E+04
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.32E+02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.74E+03
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	9.29E+02
	Chemical/Physical Properties (Continued)		
ksg (year)-1	Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	5.06E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman	B-1-1; B-2-1;	0.999

CHEMICAL-SPECIFIC INPUTS FOR AROCLOR 1016 (12674-11-2)

#### **Parameter** Reference and Explanation **Equations** Value **Biotransfer Factors for Plants** RCFRCF value was calculated by using the correlation equation with $K_{ow}$ that is cited in B-2-10 3.37E+03 Briggs (1982). Recommended value was calculated by using the $K_{ow}^{n}$ value that is provided in this table. The value was converted to a dry weight basis by using a $\mu g/g$ DW plant μg/mL soil water moisture content of 87 percent. $Br_{rootveg}$ value was calculated by dividing the RCF value with the $Kd_s$ value provided in this table. B-2-10 1.45E+01 $(\mu g/g \ DW \ plant)$ $\mu g/g$ soil B-2-9 2.91E-02 $Br_{ag}$ $Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground $(\frac{\mu g/g \ DW \ plant}{})$ produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. $\mu g/g$ soil $Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for $Br_{forage}$ B-3-9 2.91E-02 $(\frac{\mu g/g \ DW \ plant}{})$ abovegroudn produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. $\mu g/g$ soil $Bv_{ag}$ value was calculated by using the correlation equation with $K_{ov}$ and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. $Bv_{ag}$ B-2-8 7.52E+01 $(\frac{\mu g/g \ DW \ plant}{})$ $\mu g/g$ air Recommended value was calculated, for a temperature (T) of $25^{\circ}$ C, by using the H and $K_{ow}$ values that are provided in this table. $Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. B-3-8 7.52E+01 $Bv_{forage}$ $(\frac{\mu g/g \ DW \ plant}{})$ $\mu g/g$ air Recommended value was calculated, for a temperature (T) of $25^{\circ}$ C, by using the H and $K_{aw}$ values that are provided in this table. **Biotransfer Factors for Animals** Ba<sub>milk</sub> (day/kg FW) $Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in B-3-11 2.01E-03 Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. Ba<sub>beef</sub> (day/kg FW) $Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ B-3-10 6.37E-03 value that is provided in this table. Bapork (day/kg FW) $Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and B-3-12 7.71E-03 multiplying it with the $Ba_{beef}$ value. $Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value Ba<sub>egg</sub> (day/kg FW) B-3-13 2.01E+00 that is provided in this table. $Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) 5.03E-03 Bachicken (day/kg FW) B-3-14 and multiplying it with the $Ba_{beef}$ value.

#### CHEMICAL-SPECIFIC INPUTS FOR AROCLOR 1016 (12674-11-2)

Parameter	Reference and Explanation	Equations	Value
BCF <sub>fish</sub> (L/kg FW tissue)		B-4-26	NA
BAF <sub>fish</sub> (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCF$ s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCM$ s were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.33E+04
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA(1997b)	C-1-8	7.00E-05
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m³)	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	2.5E-04
Inhalation URF (µg/m³) <sup>-1</sup>		C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA = Not applicable ND = No data available

# TABLE A-3-13 CHEMICAL-SPECIFIC INPUTS FOR AROCLOR 1254 (11097-69-1)

Parameter	Reference and Explanation	Equations	Value	
Chemical/Physical Properties				
MW (g/mole)	Montgomery and Welkom (1991)		327.0	
$T_m(\mathbf{K})$	Montgomery and Welkom (1991)		283.1	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).		1.16E-07 at 25°C (liquid)	
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).		1.00E-02	
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.79E-03	
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.00E-02	
$D_w$ (cm <sup>2</sup> /s)	$D_{\rm w}$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.64E-06	
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).		1.61E+06	
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		9.98E+05	
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.83E+04	
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.37E+03	
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.93E+03	

#### CHEMICAL-SPECIFIC INPUTS FOR AROCLOR 1254 (11097-69-1)

Parameter	Reference and Explanation	Equations	Value	
Chemical/Physical Properties (Continued)				
ksg (year)-1	Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	5.06E+00	
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.993	
	Biotransfer Factors for Plants			
RCF $ (\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}) $	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then ocnverted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.40E+04	
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.42E+01	
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.00E-02	
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegorund produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.00E-02	
$Bv_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	6.01E+01	
$Bv_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	6.01E+01	
	<b>Biotransfer Factors for Animals</b>			
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.28E-02	
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	4.05E-02	

#### CHEMICAL-SPECIFIC INPUTS FOR AROCLOR 1254 (11097-69-1)

Parameter	Reference and Explanation	Equations	Value
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	4.90E-02
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.28E+01
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	3.19E-02
BCF <sub>fish</sub> (L/kg FW tissue)		B-4-26	NA
BAF <sub>fish</sub> (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCF$ s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCM$ s were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	6.66E+05
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.00E-05
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m³)	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.0E-05
<i>Inhalation URF</i> (μg/m³) <sup>-1</sup>		C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

#### Note:

NA = Not applicable ND = No data available

### CHEMICAL-SPECIFIC INPUTS FOR ARSENIC (7440-38-2)

**TABLE A-3-14** 

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		74.92		
<i>T<sub>m</sub></i> (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)		1,091 at 36 atm		
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.		0.0		
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.		0.0		
H (atm·m³/mol)	H value is assumed to be zero, because the $Vp$ and $S$ values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0		
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.07E-01		
$D_w$ (cm <sup>2</sup> /s)	$D_{\rm w}$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	1.24E-05		
$K_{ow}$ (unitless)			NA		
$K_{oc}$ (mL/g)			NA		
Kd <sub>s</sub> (mL/g)	<i>Kd<sub>s</sub></i> value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	25 at pH=4.9; 29 at pH=6.8; 31 at pH=8.0		
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	25 at pH=4.9; 29 at pH=6.8; 31 at pH=8.0		
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	25 at pH=4.9; 29 at pH=6.8; 31 at pH=8.0		
ksg (year)-1		B-1-2; B-2-2; B-3-2; B-4-2	ND		

#### CHEMICAL-SPECIFIC INPUTS FOR ARSENIC (7440-38-2)

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties (Continued)				
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0		
	Biotransfer Factors for Plants				
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$		B-2-10	ND		
$Br_{rootveg} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by multiplying the uptake slope factor with a conversion factor of 2 x $10^9$ g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for root vegetables.	B-2-10	8.00E-03		
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value for fruits was calculated by multiplying the uptake slope factor with a conversion factor of 2 x10 <sup>9</sup> g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1993e) for garden fruits. $Br_{ag}$ value for vegetables was calculated by weighting the uptake slope factors for garden fruits (75%) and leafy vegetables (25%) and multiplying the result with a conversion factor of 2 x10 <sup>9</sup> g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1993e). The weighted average $Br_{ag}$ value for aboveground produce was obtained as follows: (1) $Br_{ag}$ values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) $Br_{ag}$ values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	6.33E-03		
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by multiplying the uptake slope factor with a conversion factor of 2 x 10 <sup>9</sup> g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for leafy vegetables.	B-3-8	3.60E-02		
$Br_{grain} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{grain}$ value was calculated by multiplying the uptake slope factors with a conversion factor of 2 x 10 <sup>9</sup> g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for grains/cereals.	B-3-8	4.00E-03		
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA		
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA		

TABLE A-3-14
CHEMICAL-SPECIFIC INPUTS FOR ARSENIC (7440-38-2)

Parameter	Reference and Explanation	Equations	Value	
	Biotransfer Factors for Animals			
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	6.0E-03	
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	2.0E-03	
Ba <sub>pork</sub> (day/kg FW)		B-3-12	ND	
Ba <sub>egg</sub> (day/kg FW)		B-3-13	ND	
Ba <sub>chicken</sub> (day/kg FW)		B-3-14	ND	
BCF <sub>fish</sub> (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4.)	B-4-26	2.00E+01	
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA	
$BSAF_{fish}$ (unitless)		B-4-28	NA	
	Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	3.0E-04	
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	1.5E+00	
RfC (mg/m³)	Calculated from $\it{RfD}$ using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.1E-03	
Inhalation URF (µg/m³)-1	U.S. EPA (1997b)	C-2-1	4.3E-03	
Inhalation CSF (mg/kg/day)-1	U.S. EPA (1996d)	C-2-2	1.5E+01	

Note:

# TABLE A-3-15 CHEMICAL-SPECIFIC INPUTS FOR ATRAZINE (1912-24-9)

	Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		215.68		
$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)		444.1		
Vp (atm)	Vp value cited in Budavari, O'Neil, Smith, and Heckelman (1989)		3.66x10 <sup>-10</sup> at 25°C (solid)		
S (mg/L)	S value cited in Howard and others 1989 - 1993		3.00E+01		
<i>H</i> (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.63E-09		
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.80E-02		
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	6.03E-06		
$K_{ow}$ (unitless)	$\log K_{ow}$ value cited in Karickhoff and Long (1995).		4.07E+02		
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		1.54E+02		
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.54E+00		
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.15E+01		
	Chemical/Physical Properties (Continued)	1	1		

#### CHEMICAL-SPECIFIC INPUTS FOR ATRAZINE (1912-24-9)

Parameter	Reference and Explanation	Equations	Value	
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	6.15E+00	
ksg (year) <sup>-1</sup>	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	B-1-2; B-2-2; B-3-2; B-4-2	1.04E+01	
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $T_m$ and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.945	
	<b>Biotransfer Factors for Plants</b>			
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture ocntent of 87 percent.	B-2-10	3.00E+01	
$Br_{root  veg} $ $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.96E+01	
$Br_{ag} = \frac{(\mu g/g \ DW \ plant)}{\mu g/g \ soil}$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.20E+00	
$Br_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.20E+00	
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.28E+04	
	Biotransfer Factors for Plants (continued)			
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.28E+04	

#### CHEMICAL-SPECIFIC INPUTS FOR ATRAZINE (1912-24-9)

Parameter	Reference and Explanation	Equations	Value
	<b>Biotransfer Factors for Animals</b>		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.23E-06
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.02E-05
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.24E-05
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.23E-03
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	8.07E-06
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	5.67E+01
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.5E-02
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	2.2E-01
RfC (mg/m³)	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.2E-01
<i>Inhalation URF</i> (μg/m³) <sup>-1</sup>	Calculated from oral CSF using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-1	6.3E-05
Inhalation CSF (mg/kg/day) <sup>-1</sup>	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	2.2E-01

Note:

NA = Not applicable ND = No data available

# TABLE A-3-16 CHEMICAL-SPECIFIC INPUTS FOR BARIUM (7440-39-3)

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		137.33		
$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)		983		
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.		0.0		
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.		0.0		
H (atm·m³/mol)	${\cal H}$ value is assumed to be zero, because the ${\cal V}p$ and ${\cal S}$ values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0		
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.14E-02		
$D_w$ (cm <sup>2</sup> /s)	$D_{\rm w}$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	8.26E-06		
$K_{ow}$ (unitless)			NA		
$K_{oc}$ (mL/g)			NA		
$Kd_s$ (mL/g)	<i>Kd<sub>s</sub></i> value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0		
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0		
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value is assumed to be same as the $Kd_{s}$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0		
ksg (year) <sup>-1</sup>		B-1-2; B-2-2; B-3-2; B-4-2	ND		

#### CHEMICAL-SPECIFIC INPUTS FOR BARIUM (7440-39-3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0
	Biotransfer Factors for Plants		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$		B-2-10	ND
$Br_{rootveg} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). $Br$ values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{rootveg}$ .	B-2-10	1.50E-02
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). $Br$ values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{ag}$ (fruits). $Br_{ag}$ value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). $Br$ values for nonvegetative (reproductive) growth and $Bv$ values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for $Br_{ag}$ (vegetables). The weighted average $Br_{ag}$ value for aboveground produce was obtained as follows: (1) $Br_{ag}$ values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) $Br_{ag}$ values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	3.22E-02
$Br_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). $Bv$ values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{forage}$ .	B-3-8	1.50E-01
$Br_{grain} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{grain}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). $Br$ values for nonvegetative growth as recommended by Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{grain}$ .	B-3-8	1.50E-02
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA

# TABLE A-3-16 CHEMICAL-SPECIFIC INPUTS FOR BARIUM (7440-39-3)

Parameter	Reference and Explanation	Equations	Value
	<b>Biotransfer Factors for Animals</b>		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	3.5E-04
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	1.5E-04
Ba <sub>pork</sub> (day/kg FW)		B-3-12	ND
Ba <sub>egg</sub> (day/kg FW)	-	B-3-13	ND
Ba <sub>chicken</sub> (day/kg FW)	-	B-3-14	ND
BCF <sub>fish</sub> (L/kg FW tissue)	-	B-4-26	NA
BAF <sub>fish</sub> (L/kg FW)	-	B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	7.0E-02
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	5.0E-04
Inhalation URF (μg/m³) <sup>-1</sup>		C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

### CHEMICAL-SPECIFIC INPUTS FOR BENZALDEHYDE (100-52-7)

**TABLE A-3-17** 

$T_m$ (K) Budavari, O'Neil, Smith, and Heckelman (1989)	-Parameter	Reference and Explanation	Equations	Value
$T_m$ (K)       Budavari, O'Neil, Smith, and Heckelman (1989)		Chemical/Physical Properties		
Vp (atm)       Vp value cited in NC DEHNR (1997).       —       1.30E-03 at 25°C (solid)         S (mg/L)       S value cited in NC DEHNR (1997).       —       3.30E+03         H (atm·m³/mol)       H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.       B-1-6; B-2-6; B-2-8; B-3-6; B-2-8; B-3-6; B-4-12; B-4-19         D <sub>a</sub> (cm²/s)       D <sub>a</sub> value was obtained from CHEMDAT8 database (U.S. EPA 1994d).       B-1-6; B-2-6; B-4-12; B-4-19         D <sub>a</sub> (cm²/s)       D <sub>a</sub> value was obtained from CHEMDAT8 database (U.S. EPA 1994d).       B-1-6; B-2-6; B-3-6; B-4-6; B-4-12; B-4-19         D <sub>a</sub> (cm²/s)       D <sub>a</sub> value was obtained from CHEMDAT8 database (U.S. EPA 1994d).       B-4-20       9.48E-06         K <sub>acc</sub> (unitless)       K <sub>acc</sub> value cited in NC DEHNR (1997).       —       3.00E+01         K <sub>acc</sub> (imL/g)       K <sub>acc</sub> value was calculated by using the correlation equation with K <sub>acc</sub> for phthalates and PAHs, 'all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate K <sub>d<sub>acc</sub></sub> beast to calculate the value value was calculated by using the correlation equation with K <sub>acc</sub> that is cited in this table.	MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		106.12
$S (mg/L) \qquad S \text{ value cited in NC DEHNR (1997)}. \qquad \qquad 3.30E+03$ $H (\text{atm-m}^3/\text{mol}) \qquad H \text{ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.  D_u \text{ (cm}^3/\text{s}) \qquad D_u \text{ value was obtained from CHEMDAT8 database (U.S. EPA 1994d)}. \qquad B-1-6; B-2-6; B-3-6; B-4-6; B-3-6; B-4-6; B-3-6; B-4-6; B-3-6; B-4-6; B-3-6; B-4-6; B-3-6; B-3-6; B-4-6; B-3-6; B-4-6; B-3-6; B-3-6; B-4-6; B-3-6; B-3-6; B-3-6; B-4-6; B-3-6; B-3-6; B-3-6; B-3-6; B-3-6; B-3-6; B-3-6; B-4-6; B-3-6; B-$	$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)		329.6
H (atm·m³/mol) $H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table. $B-1-6$ ; $B-2-6$ ; $B-2-8$ ; $B-3-6$ ; $B-4-19$ ; $B-4-$	Vp (atm)	Vp value cited in NC DEHNR (1997).		at 25°C
Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table. $D_a$ (cm²/s) $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). $D_a$ value was calculated by using the correlation equation with $K_{oc}$ for phthalates, $K_{oc}$ value was calculated by using the correlation equation with $K_{oc}$ for phthalates, and $E_{oc}$ value was calculated by using the correlation equation with $E_{oc}$ for phthalates, $E_{oc}$ value was calculated by using the correlation equation with $E_{oc}$ for phthalates, $E_{oc}$ value was calculated by using the recommended $E_{oc}$ value that is provided in this table. $E_{oc}$ value was calculated by using the correlation equation with $E_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, section in soil, Recommended $E_{oc}$ value was calculated by using the $E_{oc}$ value that is provided in this table. $E_{oc}$ value was calculated by using the correlation equation with $E_{oc}$ value that is provided in this table. $E_{oc}$ value was calculated by using the correlation equation with $E_{oc}$ value that is provided in this cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment, specific to site conditions, should be used to calculate $E_{oc}$ value was calculated by using the correlation equation with $E_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment, specific to site conditions, should be used to calculate $E_{oc}$ because the value varies, depending on the fraction of organic carbon in suspended sediment, specific to site conditions, should be used to calculate $E_{oc}$ value was calculate	S (mg/L)	S value cited in NC DEHNR (1997).		3.30E+03
$D_{w} \text{ (cm}^{2}/\text{s)} \qquad D_{w} \text{ value was obtained from CHEMDAT8 database (U.S. EPA 1994d)}. \qquad B-4-20 \qquad 9.48E-06$ $K_{ow} \text{ (unitless)} \qquad K_{ow} \text{ value cited in NC DEHNR (1997)}. \qquad$	H (atm·m³/mol)	Rosenblatt (1982), which defines the constant. Recommended value was calculated	B-2-8; B-3-6; B-4-6; B-4-12;	4.18E-05
<ul> <li>K<sub>ow</sub> (unitless)</li> <li>K<sub>ow</sub> value cited in NC DEHNR (1997).</li> <li>Some value cited in NC DEHNR (1997).</li> <li>K<sub>ow</sub> (mL/g)</li> <li>K<sub>ow</sub> value was calculated by using the correlation equation with K<sub>ow</sub> for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K<sub>ow</sub> value was calculated by using the recommended K<sub>ow</sub> value that is provided in this table.</li> <li>Kd, value was calculated by using the correlation equation with K<sub>ow</sub> that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd<sub>s</sub>, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd<sub>s</sub> value was calculated by using the K<sub>ow</sub> value that is provided in this table.</li> <li>Kd<sub>sw</sub> (L/Kg)</li> <li>Kd<sub>sw</sub> value was calculated by using the correlation equation with K<sub>ow</sub> that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd<sub>sw</sub>, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd<sub>sw</sub> value was calculated by using the K<sub>ow</sub> value that is provided in this table.</li> </ul>	$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-3-6; B-4-6;	7.07E-02
$K_{oc}$ (mL/g) $K_{oc}$ (mL/g) $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. $Kd_{sw}$ (L/Kg) $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the correlation equation with $K_{sw}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.48E-06
and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. $Kd_s \text{ (cm}^3/\text{g)}$ $Kd_s \text{ value was calculated by using the correlation equation with } K_{oc} \text{ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.  Kd_{sw} \text{ (L/Kg)} Kd_{sw} \text{ value was calculated by using the correlation equation with } K_{oc} \text{ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.  Kd_{sw} \text{ (L/Kg)}$	$K_{ow}$ (unitless)	$K_{ow}$ value cited in NC DEHNR (1997).		3.00E+01
U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. $Kd_{sw} \text{ Value was calculated by using the correlation equation with } K_{oc} \text{ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.  Kd_{sw} \text{ value was calculated by using the correlation equation with } K_{oc} \text{ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.$	$K_{oc}$ (mL/g)	and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$		2.01E-01
U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	$Kd_s$ (cm <sup>3</sup> /g)	U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in	B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10;	2.01E-01
Chemical/Physical Properties (Continued)	Kd <sub>sw</sub> (L/Kg)	U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value		1.51E+00
		Chemical/Physical Properties (Continued)		

#### CHEMICAL-SPECIFIC INPUTS FOR BENZALDEHYDE (100-52-7)

-Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	8.04E-01
ksg (year)-1	Ksg value assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $T_m$ and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
	Biotransfer Factors for Plants		
RCF $ (\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}) $	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	9.50
$Br_{root  veg} \\ (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root,veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	4.72E+01
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	5.42E+00
$Br_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	5.42E+00
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	5.00E-02
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	5.00E-02

#### CHEMICAL-SPECIFIC INPUTS FOR BENZALDEHYDE (100-52-7)

-Parameter	Reference and Explanation	Equations	Value
	<b>Biotransfer Factors for Animals</b>		
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.38E-07
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	7.54E-07
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	9.12E-07
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.38E-04
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	5.95E-07
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	7.81E+00
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)	-	B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.01E-01
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m³)	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.50E-01
<i>Inhalation URF</i> (μg/m³) <sup>-1</sup>		C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA = Not applicable ND = No data available

#### CHEMICAL-SPECIFIC INPUTS FOR BENZENE (71-43-2)

Parameter	Reference and Explanation	Equations	Value			
	Chemical/Physical Properties					
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		78.11			
$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)		278.6			
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).		1.25E-01 at 25°C (liquid)			
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).		1.78E+03			
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.49E-03			
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.17E-01			
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.02E-05			
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).		137			
$K_{oc}$ (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).		6.20E+01			
<i>Kd<sub>s</sub></i> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.20E-01			
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.65E+00			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.48E+00			

#### CHEMICAL-SPECIFIC INPUTS FOR BENZENE (71-43-2)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
ksg (year) <sup>-1</sup>	Ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	3.89E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
	<b>Biotransfer Factors for Plants</b>		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.66E+01
$Br_{root veg} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	2.67E+01
$Br_{ag} = \frac{\mu g/g \ DW \ plant}{\mu g/g \ soil}$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.25E+00
$Br_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.25E+00
$Bv_{ag} = \frac{(\mu g/g \ DW \ plant)}{\mu g/g \ air}$	$Bv_{af}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.92E-03
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.92E-03
	Biotransfer Factors for Animals		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.09E-06
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.44E-06

#### CHEMICAL-SPECIFIC INPUTS FOR BENZENE (71-43-2)

Parameter	Reference and Explanation	Equations	Value
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-12	4.17E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.09E-03
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-14	2.72E-06
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.48E+01
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	Calculated from the <i>RfC</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-1-8	1.70E-02
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	2.90E-02
RfC (mg/m <sup>3</sup> )	U.S.EPA (1997e)	C-2-3	6.00E-02
<i>Inhalation URF</i> (μg/m³) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	8.30E-06
Inhalation CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	2.90E-02

Note:

NA = Not applicable ND = No data available

CHEMICAL-SPECIFIC INPUTS FOR BENZ(A)ANTHRACENE (56-55-3)

#### **Parameter** Reference and Explanation **Equations** Value **Chemical/Physical Properties** Budavari, O'Neil, Smith, and Heckelman (1989) 228.28 MW (g/mole) $T_m(\mathbf{K})$ Budavari, O'Neil, Smith, and Heckelman (1989) 433 Geometric mean value cited in U.S. EPA (1994c). 2.03E-10 Vp (atm) at 25°C (solid) S (mg/L)Geometric mean value cited in U.S. EPA (1994c). 1.28E-02 B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; $H (atm \cdot m^3/mol)$ H value was calculated by using the theoretical equation from Lyman, Reehl, and 3.62E-06 Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table. B-4-19 $D_a$ (cm<sup>2</sup>/s) $D_a$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d). B-1-6; B-2-6; 2.47E-02 B-3-6; B-4-6; B-4-21 B-4-20 $D_w$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d). 6.21E-06 $D_w$ (cm<sup>2</sup>/s) 4.77E+05 $K_{ow}$ (unitless) Geometric mean value cited in U.S. EPA (1994c). $K_{oc}$ (mL/g) Geometric mean of measured values was obtained from U.S. EPA (1996b). 2.60E + 05 $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured $Kd_s$ (mL/g) B-1-3; B-1-4; 2.60E+03B-1-5; B-1-6; B-2-3; B-2-4; organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , B-2-5; B-2-6; B-2-10; B-3-3; because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in B-3-4; B-3-5; this table. B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11 $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended 1.95E+04 $Kd_{sw}$ (L/Kg) B-4-16; B-4-18; B-4-24 sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}^{J}$ because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. $Kd_{bs}$ (mL/g) $Kd_{hs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom B-4-16; B-4-25 1.04E+04

sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate  $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended  $Kd_{bs}$  value was calculated by

using the  $K_{ac}$  value that is provided in this table.

#### CHEMICAL-SPECIFIC INPUTS FOR BENZ(A)ANTHRACENE (56-55-3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
ksg (year)-1	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.72E-01
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $S$ , $T_m$ , and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	8.81E-01
	<b>Biotransfer Factors for Plants</b>		
RCF $ \frac{(\mu g/g \ DW \ plant)}{\mu g/mL \ soil \ water} $	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis using a moisture content of 87 percent.	B-2-10	5.48E+03
$Br_{root veg} $ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root  veg}$ was calculated by dividing the <i>RCF</i> value with the $Kd_s$ value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	2.11E+00
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.02E-02
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.02E-02
$Bv_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi. (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi. (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.72E+04
$Bv_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi. (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.72E+04
	Biotransfer Factors for Animals		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.79E-03
	<u> </u>		

#### CHEMICAL-SPECIFIC INPUTS FOR BENZ(A)ANTHRACENE (56-55-3)

Parameter	Reference and Explanation	Equations	Value
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.20E-02
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-12	1.45E-02
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.79E+00
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.3 of Appendix A-3).	B-3-14	9.46E-03
BCF <sub>fish</sub> (L/kg FW tissue)		B-4-26	NA
BAF <sub>fish</sub> (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.10E+03
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)		C-1-8	ND
Oral CSF (mg/kg/day) <sup>-1</sup>	calculated by multiplying the <i>Oral CSF</i> for Benzo(a)pyrene by the relative potency factor for Benzo(a)anthracene of 0.1 (U.S.EPA 1993e)	C-1-7	7.31E-01
RfC (mg/m <sup>3</sup> )		C-2-3	ND
<i>Inhalation URF</i> (μg/m³) <sup>-1</sup>	Calculated from <i>Oral CSF</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	2.10E-04
Inhalation CSF (mg/kg/day) <sup>-1</sup>	Value based on <i>Oral CSF</i> assuming route-to-route extrapolation.	C-2-2	7.31E-01

Note:

NA = Not applicable ND = No data available

## CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)PYRENE (50-32-8)

**TABLE A-3-20** 

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		252.3
$T_m(K)$	Budavari, O'Neil, Smith, and Heckelman (1989)		452
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)		6.43E-12 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)		1.94E-03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	8.36E-07
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database in U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.18E-02
$D_w$ (cm <sup>2</sup> /s)	$D_{\rm w}$ value was obtained from CHEMDAT8 database in U.S. EPA (1994d).	B-4-20	5.85E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).		1.35E+06
$K_{oc}$ (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).		9.69E+05
$Kd_s$ (mL/g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.69E+03
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.27E+04
Kd <sub>bs</sub> (mL/g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25; B-2-10	3.87E+04

#### CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)PYRENE (50-32-8)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
ksg (year) <sup>-1</sup>	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	4.77E-01
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $S$ , $T_m$ , and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	2.65E-01
	Biotransfer Factors for Plants		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.22E+04
$Br_{root veg} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root  veg}$ value was calculated by dividing the <i>RCF</i> value with the $Kd_s$ value provided in this table (see Section A3.4.2 of Appendix A-3).	B-2-10	1.26E+00
$Br_{ag} = \frac{\mu g/g \ DW \ plant}{\mu g/g \ soil}$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.11E-02
$Br_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.11E-02
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.25E+05
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.25E+05
	Biotransfer Factors for Animals		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.07E-02
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.38E-02

#### CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)PYRENE (50-32-8)

Parameter	Reference and Explanation	Equations	Value
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 in Appendix A-3).	B-3-12	4.10E-02
$Ba_{egg}( ext{day/kg FW})$	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.07E+01
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 in Appendix A-3).	B-3-14	2.67E-02
BCF <sub>fish</sub> (L/kg, FW tissue)		B-4-26	NA
BAF <sub>fish</sub> (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	9.95E+03
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)		C-1-8	ND
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	7.30E+00
RfC (mg/m <sup>3</sup> )		C-2-3	ND
Inhalation URF (μg/m³)-1	Calculated from <i>Oral CSF</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	2.10E-03
Inhalation CSF (mg/kg/day) <sup>-1</sup>	Value based on <i>Oral CSF</i> assuming route-to-route extrapolation.	C-2-2	7.30E+00

Note:

NA = Not applicable ND = No data available

# TABLE A-3-21 CHEMICAL-SPECIFIC INPUTS FOR BENZO(B)FLUORANTHENE (205-99-2)

Parameter	Reference and Explanation	Equations	Value	
	Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)		252.32	
$T_m(\mathbf{K})$	Montgomery and Welkom (1991)		441	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)		1.06E-10 at 25°C (solid)	
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)		4.33E-03	
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.18E-06	
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.28E-02	
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-4-20	5.49E-06	
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).		1.59E+06	
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		8.36E+05	
Kd <sub>s</sub> (mL/g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.36E+03	
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.27E+04	
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.34E+04	
	Chemical/Physical Properties (Continued)			
ksg (year)-1	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	4.15E-01	

#### CHEMICAL-SPECIFIC INPUTS FOR BENZO(B)FLUORANTHENE (205-99-2)

Parameter	Reference and Explanation	Equations	Value		
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $S$ , $T_m$ , and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.822		
	<b>Biotransfer Factors for Plants</b>				
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.39E+04		
$Br_{root  veg} $ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.66E+00		
$Br_{ag} = \frac{(\mu g/g \ DW \ plant)}{\mu g/g \ soil}$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.007E-02		
$Br_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.007E-02		
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.65E+04		
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.65E+04		
	Biotransfer Factors for Animals				
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.27E-02		
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	4.00E-02		
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	4.84E-02		

#### CHEMICAL-SPECIFIC INPUTS FOR BENZO(B)FLUORANTHENE (205-99-2)

Parameter	Reference and Explanation	Equations	Value
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.27E+01
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	3.16E-02
BCF <sub>fish</sub> (L/kg FW tissue)		B-4-26	NA
BAF <sub>fish</sub> (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	9.95E+03
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)		C-1-8	ND
Oral CSF (mg/kg/day) <sup>-1</sup>	Calculated by multiplying the <i>Oral CSF</i> for Benzo(a)pyrene by the relative potency factor for Benzo(b)fluoranthene of 0.1 (U.S.EPA 1993e).	C-1-7	7.3E-01
RfC (mg/m <sup>3</sup> )		C-2-3	ND
Inhalation URF (μg/m³) <sup>-1</sup>	Calculated from <i>Oral CSF</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	2.1E-01
Inhalation CSF (mg/kg/day) <sup>-1</sup>	Value based on <i>Oral CSF</i> assuming route-to-route extrapolation.	C-2-2	7.3E-01

Note:

NA= Not applicable ND= No data available

### CHEMICAL-SPECIFIC INPUTS FOR BENZO(K)FLUORANTHENE (207-08-9)

**TABLE A-3-22** 

Parameter	Reference and Explanation	Equations	Value	
	Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)		252.32	
$T_m(\mathbf{K})$	Montgomery and Welkom (1991)		490	
Vp (atm)	U.S. EPA (1994b)		1.32E-12 at 25°C (solid)	
S (mg/L)	U.S. EPA (1994b)		8.0E-04	
H (atm·m³/mol)	$\it H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $\it MW$ , $\it S$ and $\it Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.15E-07	
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.28E-02	
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-4-20	5.49E-06	
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)		1.56E+06	
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		8.32E-05	
Kd <sub>s</sub> (mL/g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.32E+03	
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.24E+04	
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.33E+04	

#### CHEMICAL-SPECIFIC INPUTS FOR BENZO(K)FLUORANTHENE (207-08-9)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
ksg (year)-1	Ksg value was calculated by using the chemical half-life in soil, as cited in Lyman, Reehl, and Rosenblatt (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.18E-01
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $S$ , $T_m$ , and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.149
	Biotransfer Factors for Plants		
RCF $ (\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}) $	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.38E+04
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.66E+00
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.01E-02
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.01E-02
$Bv_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	5.40E+05
$Bv_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	5.40E+05
	Biotransfer Factors for Animals		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.26E-02
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.98E-02

#### CHEMICAL-SPECIFIC INPUTS FOR BENZO(K)FLUORANTHENE (207-08-9)

Parameter	Reference and Explanation	Equations	Value
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	4.82E-02
Ba <sub>egg</sub> (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.26E+01
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	3.14E-02
BCF <sub>fish</sub> (L/kg FW tissue)		B-4-26	NA
BAF <sub>fish</sub> (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	9.95E+03
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)		C-1-8	ND
Oral CSF (mg/kg/day) <sup>-1</sup>	Calculated by multiplying the <i>Oral CSF</i> for Benzo(a)pyrene by the relative potency factor for benzo(k)fluoranthene of 0.01 (U.S.EPA 1993?)	C-1-7	7.3E-02
RfC (mg/m <sup>3</sup> )		C-2-3	ND
Inhalation URF (µg/m³)-1	Calculated from <i>Oral CSF</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	2.1E-05
Inhalation CSF (mg/kg/day) <sup>-1</sup>	Value based on <i>Oral CSF</i> assuming route-to-route extrapolation.	C-2-2	7.3E-02

Note:

NA = Not applicable ND = No data available

# TABLE A-3-23 CHEMICAL-SPECIFIC INPUTS FOR BENZOIC ACID (65-85-0)

Parameter	Reference and Explanation	Equations	Value	
	Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		122.12	
$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)		395.5	
Vp (atm)	Vp value cited in U.S. EPA (1992a).	1	8.57E-06 at 25°C (solid)	
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).		3.15E+03	
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.22E-07	
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.36E-02	
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.80E-06	
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).		7.60E+01	
$K_{oc}$ (mL/g)	For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).		pH         K <sub>oc</sub> 1         31.98           2         31.80           3         30.13           4         19.81           5         4.81           6         0.99           7         0.55           8         0.50           9         0.50           10         0.50           11         0.50           12         0.50           13         0.50           14         0.50	
<i>Kd</i> <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.50E-03	

#### CHEMICAL-SPECIFIC INPUTS FOR BENZOIC ACID (65-85-0)

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties (Continued)				
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.13E-02		
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.20E-02		
ksg (year) <sup>-1</sup>	Ksg value was calculated by using the chemical half-life in soil, as cited Howard (1989-1993).	B-1-2; B-2-2; B-3-2; B-4-2	1.26E+02		
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $T_m$ and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00		
	<b>Biotransfer Factors for Plants</b>				
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.28E+01		
$Br_{root  veg} = \frac{(\mu g/g  DW  plant)}{\mu g/g  soil}$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	2.33E+03		
$Br_{ag} = \frac{\mu g/g \ DW \ plant}{\mu g/g \ soil}$	$Br_{agg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.17E+00		
$Br_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.17E+00		
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.69E+01		

#### CHEMICAL-SPECIFIC INPUTS FOR BENZOIC ACID (65-85-0)

Parameter	Reference and Explanation	Equations	Value
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.69E+01
	<b>Biotransfer Factors for Animals</b>		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	6.04E-07
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.91E-06
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.31E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	6.04E-04
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.51E-06
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.58E+01
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	4.00E+00
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m³)	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.40E+01
	Health Benchmarks (continued)		
Inhalation URF (μg/m³) <sup>-1</sup>		C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA = Not applicable ND = No data available

## CHEMICAL-SPECIFIC INPUTS FOR BENZONITRILE (100-47-0)

**TABLE A-3-24** 

Parameter	Reference and Explanation	Equations	Value	
	Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		103.12	
$T_m(K)$	Budavari, O'Neil, Smith, and Heckelman (1989)		285.85	
Vp (atm)			ND	
S (mg/L)			ND	
H (atm·m³/mol)		B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND	
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.45E-02	
$D_w$ (cm <sup>2</sup> /s)	$D_{w}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.43E-06	
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).		3.63E+01	
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		2.33E+02	
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.33E+00	
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.75E+01	
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	9.33E+00	

#### CHEMICAL-SPECIFIC INPUTS FOR BENZONITRILE (100-47-0)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
ksg (year) <sup>-1</sup>	Ksg value was assumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
Fv (unitless)	Fv value was assumed to be 1.0 due to a lack of data.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
	Biotransfer Factors for Plants		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.		1.00E+01
$Br_{root  veg} = \frac{(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})}{\mu g/g \; soil}$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	4.29E+00
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.86E+00
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.86E+00
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$		B-2-8	ND
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$		B-3-8	ND
	Biotransfer Factors for Animals	1	1
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.88E-07
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	9.12E-07

#### CHEMICAL-SPECIFIC INPUTS FOR BENZONITRILE (100-47-0)

Parameter	Reference and Explanation	Equations	Value
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.10E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.88E-04
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	7.20E-07
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	9.03E+00
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
BSAF <sub>fish</sub> (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)		C-1-8	ND
Oral CSF (mg/kg/day)-1		C-1-7	ND
RfC (mg/m³)		C-2-3	ND
Inhalation URF (µg/m³) <sup>-1</sup>		C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA = Not applicable ND = No data available

# CHEMICAL-SPECIFIC INPUTS FOR BENZYL ALCOHOL (100-51-6)

**TABLE A-3-25** 

Parameter	Reference and Explanation	Equations	Value	
Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		108.13	
$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)	-	288.29	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).		1.40E-04 at 25°C (solid)	
S (mg/L)	S value cited in U.S. EPA (1992a).	1	4.00E+04	
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.78E-07	
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.89E-02	
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.38E-06	
$K_{ow}$ (unitless)	$K_{ow}$ value cited in U.S. EPA (1995b).		1.26E+01	
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		1.02E+01	
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.02E-01	
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.66E-01	
	Chemical/Physical Properties (Continued)		-	

#### CHEMICAL-SPECIFIC INPUTS FOR BENZYL ALCOHOL (100-51-6)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.09E-01
ksg (year) <sup>-1</sup>	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $T_m$ and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
	<b>Biotransfer Factors for Plants</b>		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	7.94E+00
$Br_{root veg} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	7.77E+01
$Br_{ag} = \frac{(\mu g/g \ DW \ plant)}{\mu g/g \ soil}$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	8.95E+00
$Br_{forage} = \frac{(\mu g/g \ DW \ plant)}{\mu g/g \ soil}$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	8.95E+00
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.19E+00
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.19E+00

#### CHEMICAL-SPECIFIC INPUTS FOR BENZYL ALCOHOL (100-51-6)

Parameter	Reference and Explanation	Equations	Value
	Biotransfer Factors for Animals		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.00E-07
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.16E-07
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.83E-07
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.00E-04
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.5E-07
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.04E+00
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.00E-01
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m³)	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.10
<i>Inhalation URF</i> (μg/m³) <sup>-1</sup>		C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA = Not applicable ND = No data available

# TABLE A-3-26 CHEMICAL-SPECIFIC INPUTS FOR BENZYL CHLORIDE (100-44-7)

Parameter	Reference and Explanation	Equations	Value	
Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		126.58	
$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)		225.1	
Vp (atm)	Vp value cited in U.S. EPA (1995b).		1.60E-03 at 25°C (liquid)	
S (mg/L)	S value cited in U.S. EPA (1995b).		4.90E+02	
H (atm·m <sup>3</sup> /mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.13E-04	
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.43E-02	
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.80E-06	
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).		2.30E+00	
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		2.71E+00	
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.71E-02	
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.03E-01	
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.08E-01	
	Chemical/Physical Properties (Continued)			
ksg (year)-1	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.09E+01	
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended	B-1-1; B-2-1;	1.0	

# CHEMICAL-SPECIFIC INPUTS FOR BENZYL CHLORIDE (100-44-7)

**TABLE A-3-26** 

Parameter	Reference and Explanation	Equations	Value
	Biotransfer Factors for Plants		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.75E+00
$Br_{root veg} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	2.49E+02
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.39E+01
$Br_{forage} \\ (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.39E+01
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.28E-04
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.28E-04
	Biotransfer Factors for Animals		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.83E-08
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	5.78E-08
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	6.99E-08
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.83E-05
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	4.56E-08

#### CHEMICAL-SPECIFIC INPUTS FOR BENZYL CHLORIDE (100-44-7)

Parameter	Reference and Explanation	Equations	Value	
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.11E+00	
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA	
$BSAF_{fish}$ (unitless)		B-4-28	NA	
	Health Benchmarks			
RfD (mg/kg/day)		C-1-8	ND	
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	1.70E-01	
RfC (mg/m <sup>3</sup> )		C-2-3	ND	
<i>Inhalation URF</i> (μg/m³) <sup>-1</sup>	Calculated from <i>Oral CSF</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	4.90E-05	
Inhalation CSF (mg/kg/day) <sup>-1</sup>	Value based on <i>Oral CSF</i> assuming route-to-route extrapolation.	C-2-2	1.70E-01	

Note:

NA = Not applicable ND = No data available

# TABLE A-3-27 CHEMICAL-SPECIFIC INPUTS FOR BERYLLIUM (7440-41-7)

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		9.01		
$T_m$ (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)		1,560		
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.		0.0		
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.		0.0		
H (atm·m³/mol)	${\cal H}$ value is assumed to be zero, because the ${\cal V}p$ and ${\cal S}$ values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0		
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.39E-01		
$D_w$ (cm <sup>2</sup> /s)	$D_{\rm w}$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	5.08E-05		
$K_{ow}$ (unitless)			NA		
$K_{oc}$ (mL/g)			NA		
Kd <sub>s</sub> (mL/g)	$Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	23 at pH=4.9; 790 at pH=6.8; 1.0E+05 at pH=8.0		
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	23 at pH=4.9; 790 at pH=6.8; 1.0E+05 at pH=8.0		
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value is assumed to be same as the $Kd_{s}$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	23 at pH=4.9; 790 at pH=6.8; 1.0E+05 at pH=8.0		
ksg (year)-1		B-1-2; B-2-2; B-3-2; B-4-2	ND		

#### CHEMICAL-SPECIFIC INPUTS FOR BERYLLIUM (7440-41-7)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0
	<b>Biotransfer Factors for Plants</b>		
RCF $ (\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}) $		B-2-10	ND
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). $Br$ values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{rootveg}$ .	B-2-10	1.50E-03
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). $Br$ values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{ag}$ (fruits). $Br_{ag}$ value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). $Br$ values for nonvegetative (reproductive) growth and $Bv$ values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for $Br_{ag}$ (vegetables). The weighted average $Br_{ag}$ value for aboveground produce was obtained as follows: (1) $Br_{ag}$ values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) $Br_{ag}$ values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	2.58E-03
$Br_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). $Bv$ values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{forage}$ .	B-3-8	1.00E-02
$Br_{grain} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{grain}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). $Br$ values for nonvegetative growth as recommended by Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{grain}$ .	B-3-8	1.50E-03
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA

TABLE A-3-27
CHEMICAL-SPECIFIC INPUTS FOR BERYLLIUM (7440-41-7)

Parameter	Reference and Explanation	Equations	Value	
	Biotransfer Factors for Animals			
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	9.0E-07	
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	1.0E-03	
Ba <sub>pork</sub> (day/kg FW)		B-3-12	ND	
$Ba_{egg}$ (day/kg FW)	-	B-3-13	ND	
Ba <sub>chicken</sub> (day/kg FW)		B-3-14	ND	
BCF <sub>fish</sub> (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-4-26	4.20E+01	
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA	
$BSAF_{fish}$ (unitless)		B-4-28	NA	
	Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.00E-03	
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	4.3E+00	
RfC (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	2.0E-02	
<i>Inhalation URF</i> (μg/m³)-1	U.S. EPA (1997b)	C-2-1	2.4E-03	
Inhalation CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	8.4E+00	

Note:

#### CHEMICAL-SPECIFIC INPUTS FOR ALPHA-BHC (319-84-6)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)		290.0
$T_m(\mathbf{K})$	Montgomery and Welkom (1991)		432.2
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).		5.61E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).		2.40E+00
<i>H</i> (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.78E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	0.0191
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.04E-06
K <sub>ow</sub> (unitless)	Geometric mean value cited in U.S. EPA (1994g).		6.30E+03
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).		1.76E+03
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.76E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.32E+02
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	7.05E+01
	Chemical/Physical Properties (Continued)		
ksg (year) <sup>-1</sup>	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.87E+00
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $T_m$ and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9;	1.000

#### CHEMICAL-SPECIFIC INPUTS FOR ALPHA-BHC (319-84-6)

Parameter	Reference and Explanation	Equations	Value			
	Biotransfer Factors for Plants					
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was hen converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.02E+02			
$Br_{rootveg} \\ (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.15E+01			
$Br_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.47E-01			
$Br_{forage} $ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.47E-01			
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	9.17E+01			
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	9.17E+01			
	Biotransfer Factors for Animals					
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	5.00E-05			
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.58E-04			
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.92E-04			
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	5.00E-02			
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.25E-04			

#### CHEMICAL-SPECIFIC INPUTS FOR ALPHA-BHC (319-84-6)

Parameter	Reference and Explanation	Equations	Value
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)(see Appendix A-3).	B-4-26	4.54E+02
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)	-	B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)		C-1-8	ND
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997b)	C-1-7	6.30E+00
RfC (mg/m <sup>3</sup> )		C-2-3	ND
<i>Inhalation URF</i> (μg/m³) <sup>-1</sup>	U.S.EPA (1997b)	C-2-1	1.80E-03
Inhalation CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	6.3E+00

Note:

NA = Not applicable ND = No data available

#### CHEMICAL-SPECIFIC INPUTS FOR BETA-BHC (319-85-7)

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties				
MW (g/mole)	Montgomery and Welkom (1991)		290.83		
$T_m(\mathbf{K})$	Montgomery and Welkom (1991)		582.1		
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).		6.45E-10 at 25°C (solid)		
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).		5.42E-01		
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.46E-07		
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.9E-02		
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.40E-06		
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994g).		6.81E+03		
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).		2.14E+03		
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.14E+01		
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.60E+02		
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	8.56E+01		
	Chemical/Physical Properties (Continued)				
ksg (year)-1	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.04E+00		
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $T_m$ and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1;	0.999		

#### CHEMICAL-SPECIFIC INPUTS FOR BETA-BHC (319-85-7)

Parameter	Reference and Explanation	Equations	Value			
	Biotransfer Factors for Plants					
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.14E+02			
$Br_{rootveg} \\ (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.00E+01			
$Br_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{leafy\ veg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.36E-01			
$Br_{forage} $ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.36E-01			
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.95E+03			
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.95E+03			
	<b>Biotransfer Factors for Animals</b>					
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	5.41E-05			
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.71E-04			
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.07E-04			
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	5.41E-02			
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.35E-04			

#### CHEMICAL-SPECIFIC INPUTS FOR BETA-BHC (319-85-7)

Parameter	Reference and Explanation	Equations	Value
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). <i>BCF</i> values were obtained from U.S. EPA (1995b). <i>BCF</i> fish value cited in U.S. EPA (1995b).	B-4-26	4.82E+02
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)		C-1-8	ND
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S.EPA(1997c)	C-1-7	1.80E+00
RfC (mg/m <sup>3</sup> )		C-2-3	ND
Inhalation URF (µg/m³)-1	U.S.EPA (1997b)	C-2-1	1.80E-03
Inhalation CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	1.8E+00

Note:

NA = Not applicable ND = No data available

#### CHEMICAL-SPECIFIC INPUTS FOR BIS(2-CHLORETHYL)ETHER (111-44-4)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		143.02
$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)		223.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)		1.76E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)		1.18E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.13E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.40E-02
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.70E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c)		2.00E+01
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).		7.60E+01
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.60E-01
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.70E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.04E+00

#### CHEMICAL-SPECIFIC INPUTS FOR BIS(2-CHLORETHYL)ETHER (111-44-4)

Parameter	Reference and Explanation	Equations	Value
ksg (year) <sup>-1</sup>	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
	<b>Biotransfer Factors for Plants</b>		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.64E+00
$Br_{root veg} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.14E+01
$Br_{ag} = \frac{\mu g/g \ DW \ plant}{\mu g/g \ soil}$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	6.85E+00
$Br_{forage} = \frac{(\mu g/g \ DW \ plant)}{\mu g/g \ soil}$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	6.85E+00
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	6.37E-02
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	6.37E-02
	Biotransfer Factors for Animals		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.59E-07
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	5.02E-07
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	6.08E-07

#### CHEMICAL-SPECIFIC INPUTS FOR BIS(2-CHLORETHYL)ETHER (111-44-4)

Parameter	Reference and Explanation	Equations	Value
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.59E-04
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	3.97E-07
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	5.74E+00
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)		C-1-8	ND
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	1.1E+00
RfC (mg/m <sup>3</sup> )		C-2-3	ND
Inhalation URF (µg/m³) <sup>-1</sup>	U.S. EPA (1997e)	C-2-1	3.3E-04
Inhalation CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	1.1E+00

Note:

NA= Not applicable ND= No data available

#### CHEMICAL-SPECIFIC INPUTS FOR BROMODICHLOROMETHANE (75-27-4)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)		163.83
$T_m(\mathbf{K})$	Montgomery and Welkom (1991)		218.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).		7.68E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).		3.97E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.17E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.98E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.06E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).		1.06E+02
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		5.38E+01
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.38E-01
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.03E+00
Kd <sub>bs</sub> (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.15E+00

#### CHEMICAL-SPECIFIC INPUTS FOR BROMODICHLOROMETHANE (75-27-4)

Value
7E+01
4E+01
1E+00
1E+00
3E-03
3E-03
2E-07
6E-06
3

#### CHEMICAL-SPECIFIC INPUTS FOR BROMODICHLOROMETHANE (75-27-4)

Parameter	Reference and Explanation	Equations	Value
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	3.22E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	8.42E-04
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	2.10E-06
BCF <sub>fish</sub> (L/kg, FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.04E+01
BAF <sub>fish</sub> (L/kg FW)	1	B-4-27	NA
$BSAF_{fish}$ (unitless)	-	B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.00E-02
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	6.20E-02
RfC (mg/m³)	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.00E-02
Inhalation URF (μg/m³) <sup>-1</sup>	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-1	1.80E-05
Inhalation CSF (mg/kg/day) <sup>-1</sup>	Value based on <i>Oral CSF</i> assuming route-to-route extrapolation.	C-2-2	6.20E-02

Note:

NA = Not applicable ND = No data available

## CHEMICAL-SPECIFIC INPUTS FOR BROMOFORM (75-25-2)

**TABLE A-3-32** 

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		252.77
$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)		280.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1	7.82E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	-	3.21E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.16E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.41E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.03E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).		2.24E+02
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	-	1.26E+02
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.26E+00
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.45E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	5.04E+00

#### CHEMICAL-SPECIFIC INPUTS FOR BROMOFORM (75-25-2)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
ksg (year) <sup>-1</sup>	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
	<b>Biotransfer Factors for Plants</b>		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.13E+01
$Br_{root veg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root  veg}$ value was calculated by dividing the <i>RCF</i> value with the $Kd_s$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	1.69E+01
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.70E+00
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.70E+00
$Bv_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992) then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.89E-02
$Bv_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992) then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.89E-02
	Biotransfer Factors for Animals		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.78E-06
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	5.63E-06

#### CHEMICAL-SPECIFIC INPUTS FOR BROMOFORM (75-25-2)

Parameter	Reference and Explanation	Equations	Value
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	6.81E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.78E-03
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	4.44E-06
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.60E+01
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.00E-02
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	7.90E-03
RfC (mg/m³)	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.00E-02
Inhalation URF (μg/m³) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	1.10E-06
Inhalation CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	3.90E-03

Note:

NA = Not applicable ND = No data available

#### CHEMICAL-SPECIFIC INPUTS FOR 4-BROMOPHENYL-PHENYLETHER (101-55-3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)		249.2
$T_m(\mathbf{K})$	Montgomery and Welkom (1991)		291.8
Vp (atm)	Vp value cited in Montgomery and Welkom (1991).		1.97E-06 at 25°C (liquid)
S (mg/L)			ND
<i>H</i> (atm·m³/mol)		B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.98E-02
$D_w$ (cm <sup>2</sup> /s)	$D_{w}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	6.83E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).		1.10E+05
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		1.21E+05
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.21E+03
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.09E+03
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.85E+03
ksg (year) <sup>-1</sup>	Ksg value wasassumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman	B-1-1; B-2-1;	1.00

#### CHEMICAL-SPECIFIC INPUTS FOR 4-BROMOPHENYL-PHENYLETHER (101-55-3)

Parameter	Reference and Explanation	Equations	Value
	<b>Biotransfer Factors for Plants</b>		
RCF $ (\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}) $	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.		1.78E+03
$Br_{root veg} = \frac{(\mu g/g \ DW \ plant)}{\mu g/g \ soil}$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.47E+00
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.72E-02
$Br_{forage} = \frac{(\mu g/g \ DW \ plant)}{\mu g/g \ soil}$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.72E-02
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$		B-2-8	ND
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$		B-3-8	ND
	Biotransfer Factors for Animals	•	•
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	8.74E-04
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.76E-03
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.34E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	8.74E-01
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.18E-03
BCF <sub>fish</sub> (unitless FW tissue)		B-4-26	NA

#### CHEMICAL-SPECIFIC INPUTS FOR 4-BROMOPHENYL-PHENYLETHER (101-55-3)

Parameter	Reference and Explanation	Equations	Value
BAF <sub>fish</sub> (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.46E+04
BSAF <sub>fish</sub> (unitless)	-	B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997a)	C-1-8	5.80E-02
Oral CSF (mg/kg/day)-1		C-1-7	ND
RfC (mg/m <sup>3</sup> )	Calculated from $\it RfD$ using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	2.03E-01
Inhalation URF (µg/m³) <sup>-1</sup>	-	C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA = Not applicable ND = No data available

## CHEMICAL-SPECIFIC INPUTS FOR BUTYLBENZYLPHTHALATE (85-68-7)

**TABLE A-3-34** 

Parameter	Reference and Explanation	Equations	Value	
	Chemical/Physical Properties			
MW (g/mole)	Howard (1989-1993)		312.39	
$T_m(\mathbf{K})$	Howard (1989-1993)		238.0	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).		1.58E-08 at 25°C (liquid)	
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	-	2.58E+00	
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.91E-06	
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.65E-02	
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.17E-06	
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	-	2.59E+04	
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	-	1.37E+04	
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.37E+02	
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.03E+03	
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	5.50E+02	
ksg (year)-1	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01	

#### CHEMICAL-SPECIFIC INPUTS FOR BUTYLBENZYLPHTHALATE (85-68-7)

Parameter	Reference and Explanation	Equations	Value
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	9.64E-01
	<b>Biotransfer Factors for Plants</b>		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	5.87E+02
$Br_{root veg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	4.27E+00
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.09E-01
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.09E-01
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.46E+03
$Bv_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.46E+03
	<b>Biotransfer Factors for Animals</b>		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.06E-04
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	6.50E-04

### CHEMICAL-SPECIFIC INPUTS FOR BUTYLBENZYLPHTHALATE (85-68-7)

Parameter	Reference and Explanation	Equations	Value
	<b>Biotransfer Factors for Animals (Continued)</b>		
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	7.87E-04
Ba <sub>egg</sub> (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.06E-01
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	5.13E-04
BCF <sub>fish</sub> (L/kg FW tissue)		B-4-26	NA
BAF <sub>fish</sub> (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCF$ s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCM$ s were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	2.35E+03
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.00E-01
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m³)	Calculated from $\it{RfD}$ using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	7.00E-01
Inhalation URF (μg/m³) <sup>-1</sup>		C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA = Not applicableND = No data available

## CHEMICAL-SPECIFIC INPUTS FOR CADMIUM (7440-43-9)

**TABLE A-3-35** 

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		112.41		
$T_m$ (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)		594.1		
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.		0.0		
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.		0.0		
H (atm·m³/mol)	${\cal H}$ value is assumed to be zero, because the ${\cal V}p$ and ${\cal S}$ values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0		
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.16E-02		
$D_w$ (cm <sup>2</sup> /s)	$D_{\rm w}$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	9.45E-06		
$K_{ow}$ (unitless)			NA		
$K_{oc}$ (mL/g)			NA		
Kd <sub>s</sub> (mL/g)	<i>Kd<sub>s</sub></i> value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	15 at pH=4.9; 75 at pH=6.8; 4.3E+03 at pH=8.0		
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	15 at pH=4.9; 75 at pH=6.8; 4.3E+03 at pH=8.0		
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value is assumed to be same as the $Kd_{s}$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	15 at pH=4.9; 75 at pH=6.8; 4.3E+03 at pH=8.0		
ksg (year)-1		B-1-2; B-2-2; B-3-2; B-4-2	ND		

#### CHEMICAL-SPECIFIC INPUTS FOR CADMIUM (7440-43-9)

Description	Parameter	Reference and Explanation	Equations	Value
Description		Chemical/Physical Properties (Continued)		
$ Br_{power} = \frac{Pr_{power}}{pg'g \ DW \ plant} = \frac{Pr_{power}}{pg'g \ DW \ plant} = \frac{Pr_{power}}{pg'g \ SWI} = $	Fv (unitless)	particulate phase and zero percent in the vapor phase, as cited in	B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9;	0.0
$\frac{(\mu g/g\ DW\ plant)}{\mu g/mL\ soil\ water}$ $\frac{(\mu g/g\ DW\ plant)}{\mu g/g\ xoil}$ $\frac{Br_{roomeg}}{Br_{gas}}$ $\frac{Br_{roomeg}}{Br_$		Biotransfer Factors for Plants		
conversion factor of 2 x 10° g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for root vegetables. $ Br_{rg} V_{g} V_{$	RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$		B-2-10	ND
a conversion factor of 2 x 10° g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1993e) for garden fruits. $Br_{ag}$ value for vegetables was calculated by weighting the uptake slope factors and the conversion factor of 2 x 10° g/ha soil. The uptake slope factors and the conversion factor of 2 x 10° g/ha soil. The uptake slope factors and the conversion factor of 2 x 10° g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1993e). The weighted average $Br_{ag}$ values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) $Br_{grain}$ values for regetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day. and (2) $Br_{grain}$ values for regetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day. and (2) $Br_{grain}$ value was calculated by multiplying the uptake slope factor and the conversion factor of 2 x 10° g/ha soil. The uptake slope factor and the conversion factor of 2 x 10° g/ha soil. The uptake slope factors with a conversion factor of 2 x 10° g/ha soil. The uptake slope factors with a conversion factor of 2 x 10° g/ha soil. The uptake slope factor and the conversion factor of 2 x 10° g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for grains/cereals. $Br_{grain}$ $\frac{(\mu g/g \ DW \ plant)}{\mu g/g \ air}$ Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).  Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by multiplying the uptake slope factor with a conversion factor of 2 x $10^9$ g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for root vegetables.	B-2-10	6.40E-02
conversion factor were obtained from U.S. EPA (1992b) for leafy vegetables. $Br_{grain} = \frac{Br_{grain}}{(\frac{\mu g/g}{g})} DW \frac{B}{g} $	$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	conversion factor were obtained from U.S. EPA (1993e) for garden fruits. $Br_{ag}$ value for vegetables was calculated by weighting the uptake slope factors for garden fruits (75%) and leafy vegetables (25%) and multiplying the result with a conversion factor of $2 \times 10^9$ g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1993e).	B-2-9	1.25E-01
$\frac{(\mu g/g \ DW \ plant)}{\mu g/g \ soil}$ Conversion factor of 2 x 10° g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for grains/cereals. $Bv_{ag}$ $\frac{(\mu g/g \ DW \ plant)}{\mu g/g \ air}$ Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b). $Bv_{forage}$ $\frac{(\mu g/g \ DW \ plant)}{\mu g/g \ air}$ Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b). $B-3-8$ NA $B-3-8$ NA	$Br_{forage} \\ (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by multiplying the uptake slope factor with a conversion factor of 2 x 10 <sup>9</sup> g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for leafy vegetables.	B-3-8	3.64E-01
$\frac{(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})}{\frac{Bv_{forage}}{(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})}}{\frac{(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})}{\frac{B-3-8}{(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})}}$ Wetals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	$Br_{grain} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	conversion factor of 2 x 10 <sup>9</sup> g/ha soil. The uptake slope factor and the	B-3-8	6.20E-02
$\frac{(\mu g/g \ DW \ plant)}{\mu g/g \ air}$ U.S. EFA (1993b).	$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$		B-2-8	NA
Riotransfer Factors for Animals	$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$		B-3-8	NA
Dividuisted Factors for Annuals		Biotransfer Factors for Animals	-	

#### CHEMICAL-SPECIFIC INPUTS FOR CADMIUM (7440-43-9)

Parameter	Reference and Explanation	Equations	Value
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 20 kilograms dry weight per day and converting the result to a wet weight basis assuming a 87% moisture content in milk.	B-3-11	6.50E-06
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 20 kilograms dry weight per day and converting the result to a wet weight basis assuming a 70% moisture content in beef.	B-3-10	1.20E-04
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 4.7 kilograms dry weight per day and converting the result to a wet weight basis assuming a 70% moisture content in pork.	B-3-12	1.91E-04
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 0.2 kilograms dry weight per day and converting the result to a wet weight basis assuming a 75% moisture content in eggs.	B-3-13	2.50E-03
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 0.2 kilograms dry weight per day and converting the result to a wet weight basis assuming a 75% moisture content in chicken.	B-3-14	1.06E-01
BCF <sub>fish</sub> (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-4-26	2.50E+02
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks	_	_
RfD (water) (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.0E-04
RfD (food) (mg/kg/day)	U.S. EPA (1997b)		1.0E-03
Oral CSF (mg/kg/day) <sup>-1</sup>	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-1-7	6.3E+00
RfC (mg/m <sup>3</sup> )	Calculated from <i>RfD</i> ( <i>food</i> ) value using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.5E-03
<i>Inhalation URF</i> (μg/m³) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	1.8E-03
Inhalation CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	6.3E+00

Note:
NA = Not applicable
ND = No data available
All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

#### CHEMICAL-SPECIFIC INPUTS FOR CARBON DISULFIDE (75-15-0)

**TABLE A-3-36** 

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		76.14
$T_{m}\left(\mathbf{K}\right)$	Budavari, O'Neil, Smith, and Heckelman (1989)		161.5
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).		4.47E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).		2.67E+03
H (atm·m <sup>3</sup> /mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.27E-02
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.04E-01
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.29E-05
K <sub>ow</sub> (unitless)	Geometric mean value cited in U.S. EPA (1994c).		1.00E+02
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		5.14E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.14E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.86E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.06E+00

#### CHEMICAL-SPECIFIC INPUTS FOR CARBON DISULFIDE (75-15-0)

Chemical/Physical Properties (Continued)  Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	1
Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2;	1
	B-3-2; B-4-2	0.0
Fv value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants		
<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.44E+01
$Br_{root veg}$ value was calculated by dividing the <i>RCF</i> value with the $Kd_s$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.79E+01
$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.70E+00
$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.70E+00
$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	5.92E-04
$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	5.92E-04
Biotransfer Factors for Animals		
$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	7.94E-07
$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.51E-06
	Biotransfer Factors for Plants  RCF value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.  Br <sub>root veg</sub> value was calculated by dividing the RCF value with the $Kd_s$ value provided in this table (see section A3.4.2 of Appendix A-3).  Br <sub>oot</sub> veg value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.  Br <sub>forage</sub> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.  Br <sub>forage</sub> value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended values was calculated, for a temperature (T) of 25°C, by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for abo	value of $Fv$ was calculated by using the $Vp$ value that is provided in this table.  B-2-7; B-2-8; B-3-1; B-3-8; B-4-1; B-4-8; B-4-12; B-5-1  Biotransfer Factors for Plants  BCF value was calculated by using the correlation equation with $K_{ov}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ov}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.  BF <sub>rograver</sub> value was calculated by dividing the RCF value with the $Kd_v$ value provided in this table (see section A3.4.2 of Appendix A-3).  B-2-10  Br <sub>ograver</sub> value was calculated by using the correlation equation with $K_{ov}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ov}$ value that is provided in this table.  Br <sub>ograver</sub> value was calculated by using the correlation equation with $K_{ov}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ov}$ value that is provided in this table.  Br <sub>ograver</sub> value was calculated by using the correlation equation with $K_{ov}$ and $H$ that is cited in Bacci. Calamari, Gaggi, and Vighi (1990); and Bacci. Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the correlation equation with $K_{ov}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, Gaggi, and Vighi (1990) and Bacci (1990) and

#### CHEMICAL-SPECIFIC INPUTS FOR CARBON DISULFIDE (75-15-0)

Parameter	Reference and Explanation	Equations	Value
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	3.04E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	7.94E-04
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	1.98E-06
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.95E+01
BAF <sub>fish</sub> (L/kg FW)	-	B-4-27	NA
$BSAF_{fish}$ (unitless)	-	B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-01
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	7.00E-01
Inhalation URF (µg/m³)-1	-	C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA = Not applicable ND = No data available

#### CHEMICAL-SPECIFIC INPUTS FOR CARBON TETRACHLORIDE (56-23-5)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		153.84
$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)		250.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).		1.48E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).		7.92E+02
<i>H</i> (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.87E-02
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.56E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.77E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).		5.21E+02
$K_{oc}$ (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).		1.52E+02
<i>Kd</i> <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.52E+00
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.14E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	6.08E+00

#### CHEMICAL-SPECIFIC INPUTS FOR CARBON TETRACHLORIDE (56-23-5)

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties (Continued)				
ksg (year)-1	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.03E-01		
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0		
	<b>Biotransfer Factors for Plants</b>				
RCF $ \frac{(\mu g/g \ DW \ plant)}{\mu g/mL \ soil \ water} $	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.50E+01		
$Br_{root veg} $ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root  veg}$ value was calculated by dividing the <i>RCF</i> value with the $Kd_s$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.30E+01		
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.04E+00		
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.04E+00		
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.52E-03		
$Bv_{forage} $ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.52E-03		
	Biotransfer Factors for Animals				
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	4.14E-06		
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.30E-05		

#### CHEMICAL-SPECIFIC INPUTS FOR CARBON TETRACHLORIDE (56-23-5)

Parameter	Reference and Explanation	Equations	Value
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	1.58E-05
Ba <sub>egg</sub> (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	4.14E-03
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	1.03E-05
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). <i>BCF</i> values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	3.00E+01
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	7.00E-04
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	1.30E-01
RfC (mg/m³)	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	2.50E-03
Inhalation URF (µg/m³) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	1.50E-05
Inhalation CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	5.30E-02

Note:

NA = Not applicable ND = No data available

# TABLE A-3-38 CHEMICAL-SPECIFIC INPUTS FOR CHLORDANE (57-74-9)

	Chemical/Physical Properties					
_		Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		409.80			
$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)		381.1			
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).		3.55E-08 at 25°C (solid)			
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).		5.51E-01			
<i>H</i> (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.64E-05			
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.18E-02			
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	4.37E-06			
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).		8.66E+05			
$K_{oc}$ (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).		5.13E+04			
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.13E+02			
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.85E+03			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.05E+03			
ksg (year)-1	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.83E-01			
	Chemical/Physical Properties (Continued)	<u> </u>	1			

#### CHEMICAL-SPECIFIC INPUTS FOR CHLORDANE (57-74-9)

Parameter	Reference and Explanation	Equations	Value
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $S$ , $T_m$ , and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.997
	<b>Biotransfer Factors for Plants</b>		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.67E+03
$Br_{root veg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	1.69E+01
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.43E-02
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.43E-02
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.46E+03
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.46E+03
	<b>Biotransfer Factors for Animals</b>		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	6.88E-03
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.17E-02
	Biotransfer Factors for Animals (Continued)		
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-12	2.63E-02

#### CHEMICAL-SPECIFIC INPUTS FOR CHLORDANE (57-74-9)

Parameter	Reference and Explanation	Equations	Value
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	6.88E+00
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.3 of Appendix A-3).	B-3-14	1.72E-02
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	6.07E-01
BAF <sub>fish</sub> (L/kg FW)	-	B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.00E-01
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	3.50E-01
RfC (mg/m <sup>3</sup> )	U.S.EPA (1997b)	C-2-3	7.00E-04
Inhalation URF (μg/m³) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	1.00E-04
Inhalation CSF (mg/kg/day) <sup>-1</sup>	Value based on <i>Oral CSF</i> assuming route-to-route extrapolation.	C-2-2	3.50E-01

Note:

NA = Not applicable ND = No data available

## CHEMICAL-SPECIFIC INPUTS FOR CHLORINE (7782-50-5)

**TABLE A-3-39** 

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties				
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		71.90		
$T_m$ (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)		172.1		
Vp (atm)			ND		
S (mg/L)			ND		
H (atm·m³/mol)		B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND		
$D_a$ (cm <sup>2</sup> /s)		B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.10E-01		
$D_w$ (cm <sup>2</sup> /s)		B-4-20	1.27E-05		
$K_{ow}$ (unitless)			NA		
$K_{oc}$ (mL/g)			NA		
$Kd_s$ (mL/g)		B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	ND		
$Kd_{sw}$ (L/Kg)		B-4-16; B-4-18; B-4-24	ND		
$Kd_{bs}$ (mL/g)		B-4-16; B-4-25	ND		
ksg (year)-1		B-1-2; B-2-2; B-3-2; B-4-2	ND		
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0		

# TABLE A-3-39 CHEMICAL-SPECIFIC INPUTS FOR CHLORINE (7782-50-5)

Parameter	Reference and Explanation	Equations	Value		
	Biotransfer Factors for Plants				
RCF $(\frac{\mu g/g \ WW \ plant}{\mu g/mL \ soil \ water})$		B-2-10	ND		
$Br_{rootveg} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$		B-2-10	ND		
$Br_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$		B-2-9	ND		
$Br_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$		B-3-9	ND		
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$		B-2-8	NA		
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$		B-3-8	NA		
	Biotransfer Factors for Animals				
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all inorganics, except cadmium, mercury, selenium, and zinc.	B-3-11	1.50E-02		
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all inorganics, except cadmium, mercury, selenium, and zinc.	B-3-10	8.00E-02		
Ba <sub>pork</sub> (day/kg FW)		B-3-12	ND		
BCF <sub>egg</sub> (day/kg FW)		B-3-13	ND		
BCF <sub>chick</sub> (day/kg FW)		B-3-14	ND		
BCF <sub>fish</sub> (L/kg FW)		B-4-26	ND		
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA		
$BSAF_{fish}$ (unitless)		B-4-28	NA		

#### CHEMICAL-SPECIFIC INPUTS FOR CHLORINE (7782-50-5)

Parameter	Reference and Explanation	Equations	Value
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA 1994e or U.S. EPA 1995c	C-1-8	1.0E-01
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m <sup>3</sup> )	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.5E-01
Inhalation URF (µg/m³)-1		C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

CHEMICAL-SPECIFIC INPUTS FOR 4-CHLORO-3-METHYLPHENOL (59-50-7)

#### Parameter Reference and Explanation **Equations** Value **Chemical/Physical Properties** Budavari, O'Neil, Smith, and Heckelman (1989) 142.58 MW (g/mole) 328.6 $T_m(K)$ Budavari, O'Neil, Smith, and Heckelman (1989) ND Vp (atm) U.S.EPA (1992a) 3.85E+03S (mg/L)B-1-6; B-2-6; ND $H (atm \cdot m^3/mol)$ B-2-8; B-3-6; B-4-6; B-4-12; B-4-19 $D_a$ (cm<sup>2</sup>/s) $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). B-1-6; B-2-6; 6.96E-02 B-3-6; B-4-6; B-4-21 B-4-20 8.06E-06 $D_{w}$ (cm<sup>2</sup>/s) $D_{w}$ value was calculated using the equation cited in U.S. EPA (1996a). $K_{ow}$ (unitless) Arithmetic mean value cited in Karickhoff and Long (1995). 1.26E+03 $K_{oc}$ (mL/g) $K_{oc}$ value was calculated by using the correlation equation with $K_{ov}$ for 3.71E+03by that alter and PAHs, all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. $Kd_s$ (cm<sup>3</sup>/g) 3.71E+01 Measured organic carbon in soil, specific to site conditions, should be used to B-2-5; B-2-6; B-3-3; B-3-4; calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value B-3-5; B-3-6; that is provided in this table. B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11 $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in $Kd_{sw}$ (L/Kg) B-4-16; 2.78E+02 B-4-18; B-4-24 suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{ac}$ value that is provided in this table. $Kd_{hs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited B-4-16; B-4-25 1.48E+02 $Kd_{bs}$ (cm<sup>3</sup>/g) in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{ac}$ value that is provided in this table. **Chemical/Physical Properties (Continued)** 1.10E+01ksg (year)-1 Ksg value was calculated by using the chemical half-life in soil, as cited in B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; Lucius (1992). B-4-1; B-4-2 Fv (unitless) B-1-1; B-2-1; ND

#### CHEMICAL-SPECIFIC INPUTS FOR 4-CHLORO-3-METHYLPHENOL (59-50-7)

Parameter	Reference and Explanation	Equations	Value
	<b>Biotransfer Factors for Plants</b>		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.		6.30E+01
$Br_{rootveg} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.70E+00
$Br_{ag} = \frac{\mu g/g \ DW \ plant}{\mu g/g \ soil}$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	6.25E-01
$Br_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	6.25E-01
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$		B-2-8	ND
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$		B-3-8	ND
	Biotransfer Factors for Animals		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.00E-05
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.16E-05
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.83E-05
Ba <sub>egg</sub> (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.00E-02
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.50E-05
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.34E+02

#### CHEMICAL-SPECIFIC INPUTS FOR 4-CHLORO-3-METHYLPHENOL (59-50-7)

Parameter	Reference and Explanation	Equations	Value	
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA	
$BSAF_{fish}$ (unitless)		B-4-28	NA	
	Health Benchmarks			
RfD (mg/kg/day)		C-1-8	ND	
Oral CSF (mg/kg/day)-1		C-1-7	ND	
RfC (mg/m³)		C-2-3	ND	
Inhalation URF (µg/m³)-1		C-2-1	ND	
Inhalation CSF (mg/kg/day) <sup>-1</sup>	-	C-2-2	ND	

Note:

NA = Not applicable ND = No data available

## CHEMICAL-SPECIFIC INPUTS FOR P-CHLOROANILINE (106-47-8)

**TABLE A-3-41** 

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		127.57
$T_m(K)$	Budavari, O'Neil, Smith, and Heckelman (1989)		345.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).		3.09E-05 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).		3.36E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.17E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.80E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.02E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).		7.40E+01
$K_{oc}$ (mL/g)	For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).		K <sub>oc</sub> is 41 for pH range of 4.9 to 8
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.06E-01
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.05E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.63E+00
_	Chemical/Physical Properties (Continued)		
ksg (year)-1	Ksg value was assumed to be 0 due a a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $T_m$ and $Vp$ values that	B-1-1; B-2-1; B-2-7; B-2-8;	1.0

## CHEMICAL-SPECIFIC INPUTS FOR P-CHLOROANILINE (106-47-8)

**TABLE A-3-41** 

Parameter	Reference and Explanation	Equations	Value
	Biotransfer Factors for Plants		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.27E+01
$Br_{root veg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	3.12E+01
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.22E+00
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.22E+00
$Bv_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.66E+00
$Bv_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.66E+00
	Biotransfer Factors for Animals		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	5.88E-07
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.86E-06
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.25E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	5.88E-04
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.47E-06

#### CHEMICAL-SPECIFIC INPUTS FOR P-CHLOROANILINE (106-47-8)

Parameter	Reference and Explanation	Equations	Value	
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.55E+01	
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA	
$BSAF_{fish}$ (unitless)		B-4-28	NA	
	Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	4.00E-03	
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND	
RfC (mg/m³)	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.40E-02	
Inhalation URF (µg/m³)-1		C-2-1	ND	
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND	

Note:

NA= Not applicable ND= No data available

## CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZENE (108-90-7)

**TABLE A-3-42** 

Parameter	Reference and Explanation	Equations	Value	
	Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		112.56	
$T_m(K)$	Budavari, O'Neil, Smith, and Heckelman (1989)		228.1	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).		1.59E-02 at 25°C (liquid)	
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).		4.09E+02	
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.38E-03	
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.35E-02	
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.49E-06	
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c)		6.16E+02	
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).		2.24E+02	
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.24E+00	
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.68E+01	
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	8.96E+00	
ksg (year) <sup>-1</sup>	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.69E+00	
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0	

#### CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZENE (108-90-7)

Parameter	Reference and Explanation	Equations	Value
	<b>Biotransfer Factors for Plants</b>		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.90E+01
$Br_{root veg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.74E+01
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	9.45E-01
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	9.45E-01
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.19E-02
$Bv_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.19E-02
	<b>Biotransfer Factors for Animals</b>		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	4.89E-06
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.55E-05
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.87E-05
Ba <sub>egg</sub> (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	4.89E-03
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.22E-05
	Biotransfer Factors for Animals (Continued)		

#### **CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZENE (108-90-7)**

Parameter	Reference and Explanation	Equations	Value	
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	7.76E+01	
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA	
$BSAF_{fish}$ (unitless)		B-4-28	NA	
	Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-02	
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND	
RfC (mg/m <sup>3</sup> )	U.S. EPA (1997c)	C-2-3	2.0E-02	
Inhalation URF (µg/m³)-1		C-2-1	ND	
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND	

Note:

NA= Not applicable ND= No data available

#### CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZILATE (510-15-6)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		325.20
$T_m(\mathbf{K})$	Howard (1989-1993)		309.0
Vp (atm)	Howard (1989-1993)		2.90E-09 at 25°C (solid)
S (mg/L)	Howard (1989-1993)		1.30E+01
<i>H</i> (atm⋅m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.24E-08
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.65E-02
$D_w$ (cm <sup>2</sup> /s)	$D_{\rm w}$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	4.72E-06
K <sub>ow</sub> (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).		2.40E+04
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		3.69E+03
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.69E+01
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.77E+02
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.48E+02
	Chemical/Physical Properties (Continued)		
ksg (year)-1	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.23E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman	B-1-1; B-2-1;	8.62E-01

#### CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZILATE (510-15-6)

Parameter	Reference and Explanation	Equations	Value
	<b>Biotransfer Factors for Plants</b>		
RCF $ (\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}) $	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	5.54E+02
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.50E+01
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.14E-01
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.14E-01
$Bv_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.57E+04
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.57E+04
	Biotransfer Factors for Animals		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.91E-04
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	6.03E-04
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	7.29E-04
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.91E-01
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	4.76E-04

#### CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZILATE (510-15-6)

Parameter	Reference and Explanation	Equations	Value
BCF <sub>fish</sub> (L/kg FW tissue)		B-4-26	NA
BAF <sub>fish</sub> (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCF$ s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCM$ s were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	2.03E+03
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-02
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1995b)	C-1-7	2.7E-01
RfC (mg/m³)	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.0E-02
Inhalation URF (μg/m³) <sup>-1</sup>	U.S. EPA (1997c)	C-2-1	7.8E-06
Inhalation CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	2.7E-01

Note:

NA = Not applicable ND = No data available

#### CHEMICAL-SPECIFIC INPUTS FOR CHLORODIFLUOROMETHANE (75-45-6)

Parameter	Reference and Explanation	Equations	Value		
	Chemical/Physical Properties				
MW (g/mole)	Howard 1989-1993		86.47		
$T_m(\mathbf{K})$	Howard 1989-1993		126.6		
Vp (atm)	$\mathit{Vp}$ value cited in Howard 1989-1993.		5.63 at 25°C (liquid)		
S (mg/L)	Howard 1989-1993		2.90E+03		
<i>H</i> (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.68E-01		
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	9.72E-02		
$D_w$ (cm <sup>2</sup> /s)	$D_{\rm w}$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	1.13E-05		
$K_{ow}$ (unitless)	Calculated using the log $K_{ow}$ value cited in Howard 1989-1993.		1.20E+01		
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		9.83E+00		
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.83E-02		
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.83E-04		
	Chemical/Physical Properties (Continued)	-	•		

#### CHEMICAL-SPECIFIC INPUTS FOR CHLORODIFLUOROMETHANE (75-45-6)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.93E-01
ksg (year) <sup>-1</sup>	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) OR Howard (1989-1993) OR Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
	<b>Biotransfer Factors for Plants</b>		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	7.88E+00
$Br_{root veg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root  veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	8.01E+01
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	9.21E+00
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	9.21E+00
$Bv_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.69E-06
	Biotransfer Factors for Plants (continued)		
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.69E-06

#### CHEMICAL-SPECIFIC INPUTS FOR CHLORODIFLUOROMETHANE (75-45-6)

Parameter	Reference and Explanation	Equations	Value
	Biotransfer Factors for Animals		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	9.53E-08
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.01E-07
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.65E-07
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	9.53E-05
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.38E-07
BCF <sub>fish</sub> (L/kg, FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.89E+00
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	Calculated from <i>RfC</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-1-8	1.40E+01
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	5.00+01
<i>Inhalation URF</i> (μg/m³) <sup>-1</sup>		C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA = Not applicable ND = No data available

#### CHEMICAL-SPECIFIC INPUTS FOR CHLOROETHANE (75-00-3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		64.52
$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)		441.8
Vp (atm)	Vp value cited in Lucius et al. (1992).		159.88 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1994a)		5.74E+03
H (atm⋅m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.80
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.27E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.53E-06
$K_{ow}$ (unitless)	$K_{ow}$ value calculated from log $K_{ow}$ value cited in U.S. EPA (1995a).		1.26E+03
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		3.71E+02
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.71E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.78E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.48E+01
ksg (year) <sup>-1</sup>	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	6.72E+02
Fv (unitless)	$F_V$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_V$ was calculated by using $T_m$ and $V_p$ values that	B-1-1; B-2-1; B-2-7; B-2-8;	1.00

#### **CHEMICAL-SPECIFIC INPUTS FOR CHLOROETHANE (75-00-3)**

Parameter	Reference and Explanation	Equations	Value
	Biotransfer Factors for Plants		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then ocnverted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.30E+01
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.70E+01
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	6.25E-01
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	6.25E-01
$Bv_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	6.05E-05
$Bv_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	6.05E-05
	<b>Biotransfer Factors for Animals</b>		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.00E-05
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.16E-05
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.83E-05
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.00E-02
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.50E-05

#### **CHEMICAL-SPECIFIC INPUTS FOR CHLOROETHANE (75-00-3)**

Parameter	Reference and Explanation	Equations	Value
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.34E+02
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
RfD (mg/kg/day)	U.S.EPA (1997a)	C-1-8	4.00E-01
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	1.00E+01
Inhalation URF (µg/m³)-1		C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA = Not applicable ND = No data available

#### CHEMICAL-SPECIFIC INPUTS FOR CHLOROFORM (67-66-3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)		119.39
$T_m(\mathbf{K})$	Budavari, O'Neil, Smith, and Heckelman (1989)		209.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).		2.69E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).		7.96E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.03E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.17E-02
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.09E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).		8.90E+01
$K_{oc}$ (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).		5.30E+01
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.30E-01
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.98E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.12E+00

#### CHEMICAL-SPECIFIC INPUTS FOR CHLOROFORM (67-66-3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
ksg (year)-1	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
	<b>Biotransfer Factors for Plants</b>		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.37E+01
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the <i>RCF</i> value with the $Kd_s$ value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	2.58E+01
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.89E+00
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.89E+00
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25 °C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.65E-03
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.65E-03
	Biotransfer Factors for Animals		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	7.07E-07

#### CHEMICAL-SPECIFIC INPUTS FOR CHLOROFORM (67-66-3)

Parameter	Reference and Explanation	Equations	Value
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.23E-06
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-12	2.71E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	7.07E-04
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.3 of Appendix A-3).	B-3-14	1.76E-06
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). <i>BCF</i> values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	3.59E+00
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-02
Oral CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	6.10E-03
RfC (mg/m³)	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.50E-02
Inhalation URF (μg/m³) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	2.30E-05
Inhalation CSF (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	8.10E-02

#### Note:

NA = Not applicable ND = No data available

## CHEMICAL-SPECIFIC INPUTS FOR (BIS)-1,2-CHLOROISOPROPYLETHER (39638-32-9)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)		171.07
$T_m(\mathbf{K})$	Montgomery and Welkom (1991)		369.9
Vp (atm)	Montgomery and Welkom (1991)		7.00E-03 at 25°C (solid)
S (mg/L)	Montgomery and Welkom (1991)		1.70E+03
H (atm⋅m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.04E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.61E-02
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.38E-06
K <sub>ow</sub> (unitless)	$K_{ow}$ value cited in Howard (1989 - 1993).		3.80E+02
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		1.46E+02
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.46E+00
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.46E-02
	Chemical/Physical Properties (Continued)		

## CHEMICAL-SPECIFIC INPUTS FOR (BIS)-1,2-CHLOROISOPROPYLETHER (39638-32-9)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	5.82E+00
ksg (year) <sup>-1</sup>	Ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $T_m$ and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
	Biotransfer Factors for Plants		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.88E+01
$Br_{rootveg} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootyeg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.98E+01
$Br_{ag} = \frac{(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})}{\frac{\mu g/g \ soil}{\mu g/g \ soil}}$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.25E+00
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-9	4.44-02
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.44E-02
	<b>Biotransfer Factors for Animals</b>		
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.02E-06
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	9.55E-06

## CHEMICAL-SPECIFIC INPUTS FOR (BIS)-1,2-CHLOROISOPROPYLETHER (39638-32-9)

Parameter	Reference and Explanation	Equations	Value
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.16E-05
Ba <sub>egg</sub> (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.02E-03
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	7.54E-06
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	5.38E+01
BAF <sub>fish</sub> (L/kg FW)	-	B-4-27	NA
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	4.0E-02
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m³)	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.4E-01
Inhalation URF (μg/m³) <sup>-1</sup>		C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA = Not applicableND = No data available

#### CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORONAPHTHALENE (91-58-7)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)		162.61
$T_m(K)$	Budavari, O'Neill, Smith, and Heckelman (1989)		332.6
Vp (atm)	Vp value cited in U.S. EPA (1995b).		1.05E-05 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1995b).		1.20E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.43E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.64E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.24E-06
$K_{ow}$ (unitless)	Montgomery and Welkom (1991)		1.17E+04
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		7.14E+03
<i>Kd<sub>s</sub></i> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.14E+01
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.36E+02
Kd <sub>bs</sub> (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.86E+02
	Chemical/Physical Properties (Continued)		
ksg (year)-1	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0

#### CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORONAPHTHALENE (91-58-7)

Parameter	Reference and Explanation	Equations	Value	
Fv (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $S$ , $T_m$ , and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0	
	Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.23E+02	
$Br_{rootveg} \\ (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-9; B-2-10; B-3-9	4.51E+00	
$Br_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.72E-01	
$Br_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-10	1.72E-01	
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-9	8.46E+00	
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-9	8.46E+00	
	Biotransfer Factors for Animals			
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	9.33E-05	

#### CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORONAPHTHALENE (91-58-7)

Parameter	Reference and Explanation	Equations	Value
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.95E-04
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.57E-04
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	9.33E-02
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.33E-04
BCF <sub>fish</sub> (L/kg FW tissue)		B-4-26	NA
BAF <sub>fish</sub> (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCF$ s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	9.60E+02
$BSAF_{fish}$ (unitless)		B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997a)	C-1-8	8.00E-02
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND
RfC (mg/m³)	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	2.80E-01
Inhalation URF (μg/m³) <sup>-1</sup>		C-2-1	ND
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA = Not applicable ND = No data available

#### CHEMICAL-SPECIFIC INPUTS FOR 2-CHLOROPHENOL (95-57-8)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)		128.56
$T_m(\mathbf{K})$	Montgomery and Welkom (1991)		282.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	-	2.77E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	-	2.15E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.66E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.01E-02
$D_w$ (cm <sup>2</sup> /s)	$D_{\scriptscriptstyle W}$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.46E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).		1.45E+02
$K_{oc}$ (mL/g)	For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).		pH
Kd <sub>s</sub> (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.87E+00

#### CHEMICAL-SPECIFIC INPUTS FOR 2-CHLOROPHENOL (95-57-8)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0.	B-4-16; B-4-18; B-4-24	2.90E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0.	B-4-16; B-4-25	1.55E+01
ksg (year) <sup>-1</sup>	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
	Biotransfer Factors for Plants		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.70E+01
$Br_{rootveg} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-9; B-2-10; B-3-9	4.40E+00
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.18E+00
$Br_{forage}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-10	2.18E+00

#### CHEMICAL-SPECIFIC INPUTS FOR 2-CHLOROPHENOL (95-57-8)

Parameter	Reference and Explanation	Equations	Value	
Biotransfer Factors for Plants (Continued)				
$Bv_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-9	6.76E-01	
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	6.76E-01	
	<b>Biotransfer Factors for Animals</b>			
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.15E-06	
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.64E-06	
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	4.41E-06	
Ba <sub>egg</sub> (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.15E-03	
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.88E-06	
BCF <sub>fish</sub> (L/kg FW tissue)	<i>BCFs</i> were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.59E+01	
BAF <sub>fish</sub> (L/kg FW)		B-4-27	NA	
$BSAF_{fish}$ (unitless)		B-4-28	NA	
Health Benchmarks				
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.00E-03	
Oral CSF (mg/kg/day) <sup>-1</sup>		C-1-7	ND	
RfC (mg/m³)	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.80E-02	
Inhalation URF (µg/m³)-1		C-2-1	ND	
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND	

Note:

NA= Not applicable ND= No data available

#### CHEMICAL-SPECIFIC INPUTS FOR 2-CHLOROPHENOL (95-57-8)

## CHEMICAL-SPECIFIC INPUTS FOR 3-CHLOROPHENYL-PHENYLETHER (7005-72-3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)		204.66
$T_m(\mathbf{K})$	Montgomery and Welkom (1991)		265.1
Vp (atm)	Vp value cited in Montgomery and Welkom (1991).		3.55E-06 at 25°C (liquid)
S (mg/L)	S value cited in Montgomery and Welkom (1991).		3.30E+00
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.20E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.82E-02
$D_w$ (cm <sup>2</sup> /s)	$D_{\rm w}$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.42E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).		5.85E+04
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.		7.40E+04
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.40E+02
Kd <sub>sw</sub> (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.55E+03

## CHEMICAL-SPECIFIC INPUTS FOR 3-CHLOROPHENYL-PHENYLETHER (7005-72-3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
Kd <sub>bs</sub> (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.96E+03
ksg (year) <sup>-1</sup>	Ksg value was assumed to be zero due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
	Biotransfer Factors for Plants		
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	<i>RCF</i> value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.		1.09E+03
$Br_{rootveg} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.48E+00
$Br_{ag}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	6.80E-02
$Br_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	6.80E-02
$Bv_{ag} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.03E+01

## CHEMICAL-SPECIFIC INPUTS FOR 3-CHLOROPHENYL-PHENYLETHER (7005-72-3)

Parameter	Reference and Explanation	Equations	Value	
<b>Biotransfer Factors for Plants (Continued)</b>				
$Bv_{forage} = (\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.03E+01	
	Biotransfer Factors for Animals			
Ba <sub>milk</sub> (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	4.65E-04	
Ba <sub>beef</sub> (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.47E-03	
Ba <sub>pork</sub> (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.78E-03	
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	4.65E-01	
Ba <sub>chicken</sub> (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.16E-03	
BCF <sub>fish</sub> (L/kg FW tissue)		B-4-26	NA	
BAF <sub>fish</sub> (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	6.06E+03	
$BSAF_{fish}$ (unitless)	-	B-4-28	NA	
	Health Benchmarks			
RfD (mg/kg/day)		C-1-8	ND	
Oral CSF (mg/kg/day)-1		C-1-7	ND	
RfC (mg/m <sup>3</sup> )		C-2-3	ND	
Inhalation URF (µg/m³) <sup>-1</sup>		C-2-1	ND	
Inhalation CSF (mg/kg/day) <sup>-1</sup>		C-2-2	ND	

## CHEMICAL-SPECIFIC INPUTS FOR 3-CHLOROPHENYL-PHENYLETHER (7005-72-3)

Note:

NA = Not applicable ND = No data available